INTERACTION OF COHERENT STATES FOR HARTREE EQUATIONS

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ABSTRACT. We consider the Hartree equation with a smooth kernel and an external potential, in the semiclassical regime. We analyze the propagation of two initial wave packets, and show different possible effects of the interaction, according to the size of the nonlinearity in terms of the semiclassical parameter. We show three different sorts of nonlinear phenomena. In each case, the structure of the wave as a sum of two coherent states is preserved. However, the envelope and the center (in phase space) of these two wave packets are affected by nonlinear interferences, which are described precisely.

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1. INTRODUCTION

Consider the following Hartree equation in the semiclassical regime $\varepsilon \to 0$:

$$i\varepsilon\partial_t\psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon = V(t,x)\psi^\varepsilon + \varepsilon^\alpha \left(K * |\psi^\varepsilon|^2\right)\psi^\varepsilon, \quad t \in \mathbf{R}_+ = [0,\infty),\ x \in \mathbf{R}^d, \tag{1.1}$$

where $\alpha \geqslant 0$, $K : \mathbf{R}^d \to \mathbf{R}$, $V : \mathbf{R}_+ \times \mathbf{R}^d \to \mathbf{R}$, $d \geqslant 1$. Equation (1.1) appears for instance as a model to study superfluids, with application to Bose–Einstein condensation: in [5, 6], the kernel K is given by the formula

$$K(x) = \left(a_1 + a_2|x|^2 + a_3|x|^4\right)e^{-A^2|x|^2} + a_4 e^{-B^2|x|^2}, \quad a_1, a_2, a_3, a_4, A, B \in \mathbf{R}.$$

Assume

$$\psi^\varepsilon(0,x) = \varepsilon^{-d/4} a\left(\frac{x-q_0}{\sqrt{\varepsilon}}\right) e^{i(x-q_0)\cdot p_0/\varepsilon}, \quad a \in \mathcal{S}(\mathbf{R}^d), \quad q_0, p_0 \in \mathbf{R}^d. \tag{1.2}$$

Such initial data are called semiclassical wave packets, or coherent states. They correspond to a wave function which is equally localized in space and in frequency (at scale $\sqrt{\varepsilon}$), so

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the uncertainty principle is optimized in terms of ε: the three quantities

$$\|\psi^\varepsilon(0)\|_{L^2(\mathbf{R}^d)}, \quad \left\|\left(\sqrt{\varepsilon}\nabla - i\frac{p_0}{\sqrt{\varepsilon}}\right)\psi^\varepsilon(0)\right\|_{L^2(\mathbf{R}^d)}, \quad \text{and} \quad \left\|\frac{x-q_0}{\sqrt{\varepsilon}}\psi^\varepsilon(0)\right\|_{L^2(\mathbf{R}^d)}$$

have the same order of magnitude, $\mathcal{O}(1)$, as $\varepsilon \to 0$. In the linear case $K = 0$, another reason why such specific initial data are particularly interesting is that the superposition principle is available: if we can describe ψ^ε in the case (1.2), then the evolution of a sum of initial wave packets of the form (1.2) is simply the sum of the evolutions of each initial wave packet. In this paper, we address this question in the nonlinear setting. We describe several nonlinear interference phenomena in the case where $K \neq 0$ is smooth, and $\psi^\varepsilon(0,x)$ is the sum of two such wave packets.

The value of the parameter α in (1.1) measures the strength of the nonlinear interaction in the limit $\varepsilon \to 0$. In [12], where the Hartree nonlinearity is replaced by a local nonlinearity, it is established that if nonlinear effects are critical in terms of semiclassical dynamics (that is, the value of α is critical, see §1.2 for this notion), then despite the fact that the problem is nonlinear, the superposition principle remains valid, in the limit $\varepsilon \to 0$. In [9], the case of a homogeneous Hartree nonlinearity $K(x) = \lambda|x|^{-\gamma}$ is considered: conclusions similar to those in [12] are proven. In these two frameworks, the description of the wave packet dynamics in a "supercritical" case (nonlinear effects are stronger than in the critical case) is an open question, even on a formal level. On the other hand, in the case of a *smooth* Hartree kernel, the propagation of a single wave packet has been described in supercritical regimes ([3, 9]). In this paper, we prove that in the critical regime, nonlinear interferences affect the propagation of two initial wave packets at leading order, in contrast with the case of a homogeneous kernel. We also describe the nonlinear interactions in supercritical regimes, where even stronger interferences are present. In all cases, we prove a convergence result on all finite time intervals ($t \in [0,T]$ with T independent of ε), as $\varepsilon \to 0$.

Assumption 1.1. *The external potential V is C^3, real-valued, and at most quadratic in space:*

$$V \in C^3(\mathbf{R}_+ \times \mathbf{R}^d; \mathbf{R}), \quad \textit{and} \quad \partial_x^\beta V \in L^\infty\left(\mathbf{R}_+ \times \mathbf{R}^d\right), \quad |\beta| = 2, 3.$$

The kernel K is C^3, real-valued, bounded as well as its first three derivatives:

$$K \in C^3 \cap W^{3,\infty}(\mathbf{R}^d; \mathbf{R}).$$

Consider the Hamiltonian flow:

$$\dot{q}(t) = p(t), \;\; \dot{p}(t) = -\nabla V\left(t, q(t)\right); \quad q(0) = q_0, \; p(0) = p_0. \tag{1.3}$$

The regularity of V implies that (1.3) has a unique, global solution

$$t \mapsto (q(t), p(t)) \in C^3\left(\mathbf{R}_+; \mathbf{R}^{2d}\right).$$

Since we shall consider only bounded time intervals in this paper, the growth in time of the classical trajectories is not discussed.

1.1. **The linear case $K = 0$.** Introduce the function

$$\varphi^\varepsilon_{\rm lin}(t,x) = \varepsilon^{-d/4} u^{\rm lin}\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}\right) e^{i(S(t)+p(t)\cdot(x-q(t)))/\varepsilon},$$

where (q,p) is given by (1.3), the classical action is given by

$$S(t) = \int_0^t \left(\frac{1}{2}|p(s)|^2 - V(s, q(s))\right) ds, \tag{1.4}$$

and the envelope $u^{\rm lin} = u^{\rm lin}(t,y)$ solves

$$i\partial_t u^{\rm lin} + \frac{1}{2}\Delta u^{\rm lin} = \frac{1}{2}\left\langle y, \nabla^2 V\left(t, q(t)\right) y\right\rangle u^{\rm lin} \quad ; \quad u^{\rm lin}(0,y) = a(y), \tag{1.5}$$

where the notation ∇^2 stands for the Hessian matrix, and since the space variable for $u^{\rm lin}$ is y, Δ stands for Δ_y. The following lemma is standard, see e.g. [4, 13, 14, 15, 24, 25, 26] and references therein.

Lemma 1.2. *Let $a \in \mathcal{S}(\mathbf{R}^d)$, and ψ^ε solve* (1.1) *with $K = 0$, and* (1.2)*. There exist positive constants C and C_1 independent of ε such that*

$$\|\psi^\varepsilon(t) - \varphi^\varepsilon_{\rm lin}(t)\|_{L^2(\mathbf{R}^d)} \leqslant C\sqrt{\varepsilon}e^{C_1 t}, \quad \forall t \geqslant 0.$$

In particular, there exists $c > 0$ independent of ε such that

$$\sup_{0\leqslant t\leqslant c\ln\frac{1}{\varepsilon}} \|\psi^\varepsilon(t) - \varphi^\varepsilon_{\rm lin}(t)\|_{L^2(\mathbf{R}^d)} \underset{\varepsilon\to 0}{\longrightarrow} 0.$$

1.2. **Nonlinear case: notion of criticality.** In the nonlinear case $K \neq 0$, the following distinction was established in [9]:

- If $\alpha > 1$, nonlinear effects are negligible at leading order: with the same function $\varphi^\varepsilon_{\rm lin}$ as in the previous section, there exists $C > 0$ such that
$$\|\psi^\varepsilon(t) - \varphi^\varepsilon_{\rm lin}(t)\|_{L^2(\mathbf{R}^d)} \leqslant C\sqrt{\varepsilon}e^{Ct}, \quad \forall t \geqslant 0.$$
- If $\alpha = 1$, nonlinear effects become relevant at leading order (unless $K(0) = 0$): there exists $C > 0$ such that
$$\left\|\psi^\varepsilon(t) - \varphi^\varepsilon_{\rm lin}(t)e^{-itK(0)\|a\|^2_{L^2}}\right\|_{L^2(\mathbf{R}^d)} \leqslant C\sqrt{\varepsilon}e^{Ct}, \quad \forall t \geqslant 0.$$

From this point of view, the case $\alpha = 1$ is critical: the supercritical behavior is described in two cases, $\alpha = 1/2$ ([9]) and $\alpha = 0$ ([3, 9]). The approximate solution derived in these two cases may be viewed as a particular case of the approximate solution presented below, when one of the two initial wave packets is zero, so we choose not to be more explicit about these two cases here. Other cases could be described as well: the case $\alpha \in (0, 1/2)$ is similar to the case $\alpha = 0$, and the case $\alpha \in (1/2, 1)$ is similar to the case $\alpha = 1/2$, up to several modifications in the notations essentially.

In the case $\alpha > 1$, nonlinear effects are negligible at leading order, so the superposition principle remains: the nonlinear evolution of two (or more) initial wave packets is well approximated by the sum of the linear evolutions of each wave packet. We will see that when $\alpha \leqslant 1$, nonlinear interferences affect the behavior of ψ^ε at leading order.

Throughout this paper, for $k \in \mathbf{N}$, we will denote by

$$\Sigma^k = \left\{ f \in L^2(\mathbf{R}^d)\ ;\ \|f\|_{\Sigma^k} := \sum_{|\alpha|+|\beta|\leqslant k} \left\|x^\alpha \partial_x^\beta f\right\|_{L^2(\mathbf{R}^d)} < \infty \right\},$$

and $\Sigma^1 = \Sigma$. As established in [9], if $\psi^\varepsilon(0,\cdot) \in L^2(\mathbf{R}^d)$, then under Assumption 1.1, (1.1) has a unique solution $\psi^\varepsilon \in C(\mathbf{R}_+; L^2(\mathbf{R}^d))$, regardless of the value of α[1], and

$$\|\psi^\varepsilon(t)\|_{L^2(\mathbf{R}^d)} = \|\psi^\varepsilon(0)\|_{L^2(\mathbf{R}^d)}, \quad \forall t \geqslant 0.$$

[1]To be complete, the regularity assumption on V in [9] is stronger, but Assumption 1.1 is enough.

1.3. **Critical case:** $\alpha = 1$**.** We now consider (1.1) in the case of two initial wave packets: (1.2) is replaced by

$$\psi^\varepsilon(0,x) = \varepsilon^{-d/4} \sum_{j=1,2} a_j \left(\frac{x-q_{j0}}{\sqrt{\varepsilon}}\right) e^{i(x-q_{j0})\cdot p_{j0}/\varepsilon}, \tag{1.6}$$

with $(q_{10}, p_{10}) \neq (q_{20}, p_{20})$. Let (q_j, p_j) be the solution to (1.3) with initial data (q_{j0}, p_{j0}), and S_j the associated classical action given by (1.4). Define the approximate solution as

$$\psi^\varepsilon_{\rm app}(t,x) = \varepsilon^{-d/4} \sum_{j=1,2} u_j \left(t, \frac{x-q_j(t)}{\sqrt{\varepsilon}}\right) e^{i(S_j(t)+p_j(t)\cdot(x-q_j(t)))/\varepsilon}, \tag{1.7}$$

where the envelopes u_j are given by the formulas:

$$\begin{cases} u_1(t,y) = u_1^{\rm lin}(t,y) e^{-itK(0)\|a_1\|^2_{L^2} - i\|a_2\|^2_{L^2}\int_0^t K(q_1(s)-q_2(s))ds}, \\ u_2(t,y) = u_2^{\rm lin}(t,y) e^{-itK(0)\|a_2\|^2_{L^2} - i\|a_1\|^2_{L^2}\int_0^t K(q_2(s)-q_1(s))ds}, \end{cases} \tag{1.8}$$

with obvious notations adapted from (1.5).

Theorem 1.3. *Let $d \geqslant 1$, V, K satisfying Assumption 1.1. Let $a_1, a_2 \in \Sigma^3$, and ψ^ε be the solution to* (1.1) *with $\alpha = 1$ and initial data* (1.6)*. Then for any $T > 0$ independent of ε, there exists $C > 0$ independent of ε such that*

$$\sup_{t\in[0,T]} \left\|\psi^\varepsilon(t) - \psi^\varepsilon_{\rm app}(t)\right\|_{L^2(\mathbf{R}^d)} \leqslant C\sqrt{\varepsilon},$$

where $\psi^\varepsilon_{\rm app}$ is given by (1.7)–(1.8)*.*

The nonlinear effects are described at leading order by the exponentials in (1.8). Even in the case of a single initial wave packet (say $a_2 = 0$), the nonlinearity affects the envelope by a phase self-modulation. The second terms in the exponentials describe the effect of nonlinear interferences, which are not a simple superposition in general.

As pointed out above, it may be surprising to notice that even in the critical case $\alpha = 1$, nonlinear interferences are present at leading order. This is in sharp contrast with the case of an homogeneous kernel, $K(x) = \lambda|x|^{-\gamma}$, $0 < \gamma < \min(2,d)$. It was shown in [9] that in this case, the critical value for α is $\alpha_c = 1 + \gamma/2$, and that when $\alpha = \alpha_c$, the superposition principle remains, even though the nonlinearity affects the propagation of a single wave packet at leading order (the envelope equation is nonlinear).

1.4. **Case** $\alpha = 1/2$**.** The approximate solution is now constructed as follows. The pairs (q_j, p_j), $j = 1, 2$, are still given by the usual classical flow (1.3). On the other hand, we modify the actions, and make them ε-dependent:

$$\begin{cases} S_1^\varepsilon(t) = \displaystyle\int_0^t \left(\frac{1}{2}|p_1(s)|^2 - V(s,q_1(s))\right) ds \\ \qquad - t\sqrt{\varepsilon}K(0)\|a_1\|^2_{L^2(\mathbf{R}^d)} - \sqrt{\varepsilon}\|a_2\|^2_{L^2(\mathbf{R}^d)} \displaystyle\int_0^t K\left(q_1(s)-q_2(s)\right) ds, \\ S_2^\varepsilon(t) = \displaystyle\int_0^t \left(\frac{1}{2}|p_2(s)|^2 - V(s,q_2(s))\right) ds \\ \qquad - t\sqrt{\varepsilon}K(0)\|a_2\|^2_{L^2(\mathbf{R}^d)} - \sqrt{\varepsilon}\|a_1\|^2_{L^2(\mathbf{R}^d)} \displaystyle\int_0^t K\left(q_2(s)-q_1(s)\right) ds. \end{cases} \tag{1.9}$$

Consider the system of Schrödinger equations

$$
\begin{cases}
i\partial_t \tilde u_1 + \frac{1}{2}\Delta \tilde u_1 = \frac{1}{2}\left\langle y, \nabla^2 V\left(t, q_1(t)\right) y\right\rangle \tilde u_1 + \|a_1\|^2_{L^2} y\cdot \nabla K(0)\tilde u_1 \\
\qquad\qquad\qquad + \|a_2\|^2_{L^2} y\cdot \nabla K\left(q_1(t)-q_2(t)\right)\tilde u_1, \\
i\partial_t \tilde u_2 + \frac{1}{2}\Delta \tilde u_2 = \frac{1}{2}\left\langle y, \nabla^2 V\left(t, q_2(t)\right) y\right\rangle \tilde u_2 + \|a_2\|^2_{L^2} y\cdot \nabla K(0)\tilde u_2 \\
\qquad\qquad\qquad + \|a_1\|^2_{L^2} y\cdot \nabla K\left(q_2(t)-q_1(t)\right)\tilde u_2,
\end{cases} \tag{1.10}
$$

with initial data a_1 and a_2, respectively. These are two linear equations with time dependent potentials, which are polynomial in y, of degree (at most) two. The following result is classical, see e.g. [36, 17, 18]:

Lemma 1.4. *For $j=1,2$, let $a_j\in L^2(\mathbf{R}^d)$, and $(q_j,p_j)\in C^3(\mathbf{R}_+;\mathbf{R}^{2d})$ given by* (1.3)*. There exists a unique solution $(\tilde u_1,\tilde u_2)\in C(\mathbf{R}_+;L^2(\mathbf{R}^d))^2$ to* (1.10) *such that $(\tilde u_1,\tilde u_2)_{|t=0}=(a_1,a_2)$. In addition, the following conservations hold:*

$$
\|\tilde u_j(t)\|_{L^2(\mathbf{R}^d)} = \|a_j\|_{L^2(\mathbf{R}^d)}, \quad \forall t\geqslant 0,\ j=1,2.
$$

To define the envelopes in (1.7), set

$$
\begin{aligned}
u_1(t,y_1) &= \tilde u_1(t,y_1)\exp\left(i\int_0^t \Big(\nabla K(0)\cdot \tilde G_1(s) + \nabla K\left(q_1(s)-q_2(s)\right)\cdot \tilde G_2(s)\Big)\,ds\right),\\
u_2(t,y_2) &= \tilde u_2(t,y_2)\exp\left(i\int_0^t \Big(\nabla K(0)\cdot \tilde G_2(s) + \nabla K\left(q_2(s)-q_1(s)\right)\cdot \tilde G_1(s)\Big)\,ds\right),
\end{aligned} \tag{1.11}
$$

where $\tilde G_j(t) = \displaystyle\int_{\mathbf{R}^d} z|\tilde u_j(t,z)|^2dz$. Since $\tilde G_j$ is a nonlinear function of $\tilde u_j$, the system formed by (u_1,u_2) is nonlinear, with a nonlinear coupling: nonlinear interferences are present both in rapid oscillations — the modified actions generate $\sqrt{\varepsilon}$-oscillations in time — and in the envelopes. The presence of the functions $\tilde G_j$ in the above formulas reveals non-local (in space) nonlinear phenomena concerning the envelopes in $\psi^\varepsilon_{\rm app}$. Since the problem is now supercritical, it should not be surprising that stronger regularity properties are assumed in the following result (see Remark 4.2).

Theorem 1.5. *Let $d\geqslant 1$. Assume that V and K are real-valued and satisfy:*

$$
V\in C^5(\mathbf{R}_+\times\mathbf{R}^d;\mathbf{R}), \quad \textit{and} \quad \partial_x^\beta V\in L^\infty\left(\mathbf{R}_+\times\mathbf{R}^d\right), \quad 2\leqslant|\beta|\leqslant 5.
$$
$$
K\in W^{5,\infty}(\mathbf{R}^d;\mathbf{R}).
$$

Let $a_1,a_2\in\Sigma^5$, and $\psi^\varepsilon_{\rm app}$ be given by (1.7)–(1.9)–(1.10)–(1.11)*. Then for any $T>0$ independent of ε, there exists $C>0$ independent of ε such that*

$$
\sup_{t\in[0,T]}\left\|\psi^\varepsilon(t)-\psi^\varepsilon_{\rm app}(t)\right\|_{L^2(\mathbf{R}^d)}\leqslant C\sqrt{\varepsilon}.
$$

1.5. **Case $\alpha=0$.** In this last case, nonlinear interferences affect even the geometric properties of the wave packets, in contrast with the cases $\alpha=1$ and $\alpha=1/2$. The trajectories are required to evolve according to the system

$$
\begin{cases}
\dot q_1(t) = p_1(t),\\
\dot p_1(t) = -\nabla V\left(t,q_1(t)\right) - \|a_1\|^2_{L^2}\nabla K(0) - \|a_2\|^2_{L^2}\nabla K\left(q_1(t)-q_2(t)\right),\\
\dot q_2(t) = p_2(t),\\
\dot p_2(t) = -\nabla V\left(t,q_2(t)\right) - \|a_2\|^2_{L^2}\nabla K(0) - \|a_1\|^2_{L^2}\nabla K\left(q_2(t)-q_1(t)\right).
\end{cases} \tag{1.12}
$$

Unless ∇K is a constant (which would implies that K is constant, a trivial case), one cannot decouple the unknowns (q_1, p_1) and (q_2, p_2): the coupling cannot by undone, and the "good unknown" is $(q_1, p_1, q_2, p_2) \in \mathbf{R}^{4d}$. In view of Assumption 1.1, Cauchy–Lipschitz Theorem implies:

Lemma 1.6. *For $j = 1, 2$, let $(q_{j0}, p_{j0}) \in \mathbf{R}^{2d}$. If V and K satisfy Assumption 1.1, then* (1.12) *has a unique solution $(q_1, p_1, q_2, p_2) \in C^3(\mathbf{R}_+; \mathbf{R}^{4d})$.*

Remark 1.7 (Hamiltonian structure). If the external potential V does not depend on time, $\partial_t V = 0$, and the kernel K is even, $K(-x) = K(x)$ for all $x \in \mathbf{R}^d$, then the Hartree equation (1.1) has a Hamiltonian structure. In the case $\alpha = 0$, the following energy is independent of t,

$$\frac{\varepsilon^2}{2}\|\nabla\psi^\varepsilon(t)\|_{L^2}^2 + \int_{\mathbf{R}^d} V(x)|\psi^\varepsilon(t,x)|^2 dx + \frac{1}{2}\iint_{\mathbf{R}^{2d}} K(x-y)|\psi^\varepsilon(t,y)|^2|\psi^\varepsilon(t,x)|^2 dxdy.$$

Note that since K is even, $\nabla K(0) = 0$, and $\nabla K(q_2 - q_1) = -\nabla K(q_1 - q_2)$. In that case, the system of modified trajectories (1.12) is also Hamiltonian, as can be seen from the approach presented in [21]. Given the state variable $z = (q_1, p_1, q_2, p_2)^T$, let

$$H(t,z) = \alpha_1\left(\frac{1}{2}|p_1|^2 + V(q_1)\right) + \alpha_2\left(\frac{1}{2}|p_2|^2 + V(q_2)\right) + \alpha_1\alpha_2 K\left(q_1 - q_2\right),$$

where $\alpha_j = \|a_j\|_{L^2}^2$. The system (1.12) has the Hamiltonian structure

$$\frac{dz}{dt} = JD_zH(t,z) \quad \text{with} \quad J = \begin{pmatrix} 0 & 1/\alpha_1 & 0 & 0 \\ -1/\alpha_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/\alpha_2 \\ 0 & 0 & -1/\alpha_2 & 0 \end{pmatrix}.$$

One checks indeed that the function H is conserved along solutions of (1.12).

Before defining the modified actions, we have to construct also the envelopes. Consider the coupled, nonlinear system

$$\left\{\begin{aligned} &i\partial_t u_1 + \frac{1}{2}\Delta u_1 = \frac{1}{2}\langle y, M_1(t)y\rangle u_1 - \left\langle \nabla^2 K(0)G_1(t), y\right\rangle u_1 \\ &\quad - \left\langle \nabla^2 K(q_1 - q_2)G_2(t), y\right\rangle u_1 + \frac{1}{2}\left(\int \left\langle z, \nabla^2 K(0)z\right\rangle |u_1(t,z)|^2 dz\right) u_1 \\ &\quad + \frac{1}{2}\left(\int \left\langle z, \nabla^2 K(q_1 - q_2)z\right\rangle |u_2(t,z)|^2 dz\right) u_1, \\ &i\partial_t u_2 + \frac{1}{2}\Delta u_2 = \frac{1}{2}\langle y, M_2(t)y\rangle u_2 - \left\langle \nabla^2 K(0)G_2(t), y\right\rangle u_2 \\ &\quad - \left\langle \nabla^2 K(q_2 - q_1)G_1(t), y\right\rangle u_2 + \frac{1}{2}\left(\int \left\langle z, \nabla^2 K(0)z\right\rangle |u_2(t,z)|^2 dz\right) u_2 \\ &\quad + \frac{1}{2}\left(\int \left\langle z, \nabla^2 K(q_2 - q_1)z\right\rangle |u_1(t,z)|^2 dz\right) u_2, \end{aligned}\right. \tag{1.13}$$

where the functions q_j are assessed at time t, and we have denoted

$$G_j(t) = \int_{\mathbf{R}^d} z|u_j(t,z)|^2 dz, \quad j = 1,2, \tag{1.14}$$

$$M_1(t) = \|a_1\|^2_{L^2(\mathbf{R}^d)} \nabla^2 K(0) + \|a_2\|^2_{L^2(\mathbf{R}^d)} \nabla^2 K\left(q_1(t) - q_2(t)\right) + \nabla_x^2 V\left(t, q_1(t)\right), \tag{1.15}$$

$$M_2(t) = \|a_2\|^2_{L^2(\mathbf{R}^d)} \nabla^2 K(0) + \|a_1\|^2_{L^2(\mathbf{R}^d)} \nabla^2 K\left(q_2(t) - q_1(t)\right) + \nabla_x^2 V\left(t, q_2(t)\right). \tag{1.16}$$

The system defining the envelopes is more nonlinear than the cases $\alpha = 1$ and $\alpha = 1/2$, and, as in the case $\alpha = 1/2$, involves nonlinear terms which are non-local in space. In Section 5, we prove the following result:

Proposition 1.8. *Let (q_1, p_1, q_2, p_2) be given by Lemma 1.6, and $a_1, a_2 \in \Sigma^k$ with $k \geqslant 1$. Then* (1.13) *has a unique solution $(u_1, u_2) \in C(\mathbf{R}_+; \Sigma^k)$ with initial data (a_1, a_2). In addition, the following conservations hold:*

$$\|u_j(t)\|_{L^2(\mathbf{R}^d)} = \|a_j\|_{L^2(\mathbf{R}^d)}, \quad \forall t \geqslant 0,\ j = 1,2.$$

We can then define the modified, ε-dependent actions:

$$\begin{aligned} S_1^\varepsilon(t) = \int_0^t \Big(&\frac{1}{2}|p_1(s)|^2 - V\left(s, q_1(s)\right) - K(0)\|a_1\|^2_{L^2} - K\left(q_1(s) - q_2(s)\right)\|a_2\|^2_{L^2} \\ &+ \sqrt{\varepsilon}\nabla K(0) \cdot G_1(s) + \sqrt{\varepsilon}\nabla K\left(q_1(s) - q_2(s)\right) \cdot G_2(s)\Big) ds, \\ S_2^\varepsilon(t) = \int_0^t \Big(&\frac{1}{2}|p_2(s)|^2 - V\left(s, q_2(s)\right) - K(0)\|a_2\|^2_{L^2} - K\left(q_2(s) - q_1(s)\right)\|a_1\|^2_{L^2} \\ &+ \sqrt{\varepsilon}\nabla K(0) \cdot G_2(s) + \sqrt{\varepsilon}\nabla K\left(q_2(s) - q_1(s)\right) \cdot G_1(s)\Big) ds. \end{aligned}$$

Theorem 1.9. *Let $d \geqslant 1$. Assume that V and K are real-valued and satisfy:*

$$V \in C^7(\mathbf{R}_+ \times \mathbf{R}^d; \mathbf{R}), \quad \textit{and} \quad \partial_x^\beta V \in L^\infty\left(\mathbf{R}_+ \times \mathbf{R}^d\right), \quad 2 \leqslant |\beta| \leqslant 7.$$
$$K \in W^{7,\infty}(\mathbf{R}^d; \mathbf{R}).$$

Let $a_1, a_2 \in \Sigma^7$. There exist $\theta_1, \theta_2 \in C^2(\mathbf{R}_+; \mathbf{R})$, with $\theta_j(0) = \dot\theta_j(0) = 0$, such that the following holds. For any $T > 0$ independent of ε, there exists $C > 0$ independent of ε such that

$$\sup_{t \in [0,T]} \Big\| \psi^\varepsilon(t) - \sum_{j=1,2} \varphi_j^\varepsilon(t) e^{i\theta_j(t)} \Big\|_{L^2(\mathbf{R}^d)} \leqslant C\sqrt{\varepsilon},$$

where we have denoted $\varphi_j^\varepsilon(t,x) = \varepsilon^{-d/4} u_j\left(t, \frac{x - q_j(t)}{\sqrt{\varepsilon}}\right) e^{i\left(S_j^\varepsilon(t) + p_j(t)\cdot(x - q_j(t))\right)/\varepsilon}$.

In general, the phase shifts θ_j are not identically zero. In Section 8, we give the expression of these functions, which is probably a bit too involved to present at this stage (see Equation (8.4)), and check that in general, $(\ddot\theta_1(0), \ddot\theta_2(0)) \neq (0,0)$. Such modifications do not appear in the case of a single wave packet studied in [3, 9]. Technically, the reason is two-fold. First, in [3, 9], it is assumed that $\nabla K(0) = 0$, so the first line in (8.4) vanishes. Then, the second line in (8.4) accounts for the presence of two wave packets, and measures some coupling through a phase modulation: it vanishes in the case of a single wave packet.

1.6. **Comments.**

The results. In the three cases studied here, the interferences are nonlinear. They always affect the envelopes. In the case $\alpha = 1/2$, they affect moreover the action, and in the case $\alpha = 0$, the system (1.12) reveals a nonlinear coupling of the trajectories, so all the terms involved in $\psi^\varepsilon_{\rm app}$ are influenced by the nonlinearity. Our results are original even in the case $V = 0$.

Nonlinear interferences always carry a non-local in time aspect. Even if K is decaying at infinity, the interactions ignore the mutual distance of the two wave packets: no matter how large $q_1(t) - q_2(t)$ is, nonlinear interferences affect the solution at order $\mathcal{O}(1)$ on finite time intervals, as $\varepsilon \to 0$.

Our results yield a unified picture concerning Wigner measures (see e.g. [8, 20, 32]):

Corollary 1.10. *In all the cases $\alpha = 1$, $\alpha = 1/2$ and $\alpha = 0$, and under the Assumptions of Theorem 1.3, Theorem 1.5 and Theorem 1.9, respectively, the Wigner measure of ψ^ε is given by*

$$w(t,x,\xi) = \sum_{j=1,2} \|a_j\|^2_{L^2(\mathbf{R}^d)} \delta\left(x - q_j(t)\right) \otimes \delta\left(\xi - p_j(t)\right),$$

with (q_j, p_j) given by the standard Hamiltonian flow (1.3) *in the cases $\alpha = 1$ and $\alpha = 1/2$, and (q_1, p_1, q_2, p_2) given by* (1.12) *in the case $\alpha = 0$.*

To be complete, the proof of this corollary relies also on the results established in Section 3. In the two cases $\alpha = 1$ and $\alpha = 1/2$, the Wigner measure of $\psi^\varepsilon_{\rm app}$ is not affected by the nonlinearity, even though we have seen that the Hartree nonlinearity does affect the leading order behavior of the wave function, and that nonlinear exchanges are present at leading order. In the case $\alpha = 0$, nonlinear effects alter the Wigner measure, *even when* $\nabla K(0) = 0$, a case which is often encountered in Physics (typically, $K(-x) = K(x)$, so the Hartree nonlinearity has an Hamiltonian structure). In other words, the Wigner measure of ψ^ε is always affected by nonlinear interferences. This is in contrast with the case of a single initial wave packet, where the trajectory (q,p) is modified as if an electric field $\|a\|^2_{L^2} \nabla K(0) \cdot x$ was added to the initial Hamiltonian $-\frac{1}{2}\Delta + V$: if $\nabla K(0) = 0$, then the Wigner measure ignores nonlinear effect even in the case $\alpha = 0$ (see [3, 9]).

Note that if $\nabla K(0) \neq 0$ (a case which is not necessarily physically relevant, from the above remark), Theorem 1.9 is new *even in the case of a single wave packet*.

In this paper, we treat the case of two initial wave packets: our approach can easily be generalized to any (finite) number of initial wave packets, the main difference being that formulas get more and more involved as the number of initial wave packets increases (but the main analytical aspects are essentially the same).

We have examined the leading order behavior of the exact solution, up to an error of order $\mathcal{O}(\sqrt{\varepsilon})$: like in [3], ψ^ε could be approximated by a series involving powers of $\sqrt{\varepsilon}$, up to arbitrary order. This statement is made more precise in §8 (see in particular Equation (8.2)): to prove Theorem 1.9, the asymptotic expansion of the main unknown functions has to be pushed one step further than in the cases $\alpha = 1$ and $\alpha = 1/2$.

Comparison with related works. We briefly give more details concerning the propagation of two wave packets described in [9, 12]. Since both cases are rather similar, we describe the case of a Hartree nonlinearity only ([9]). The main difference in the setting is that (1.1) is replaced with

$$i\varepsilon\partial_t \psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon = V(t,x)\psi^\varepsilon + \lambda\varepsilon^\alpha \left(|x|^{-\gamma} * |\psi^\varepsilon|^2\right)\psi^\varepsilon, \quad t \geqslant 0,\ x \in \mathbf{R}^d,$$

with $\lambda \in \mathbf{R}$ and $0 < \gamma < \min(2, d)$. The critical value for α is $\alpha_c = 1 + \gamma/2 > 1$. When $\alpha = \alpha_c$, the propagation of one initial wave packet is well approximated by

$$\varphi^\varepsilon(t,x) = \varepsilon^{-d/4} u\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}\right) e^{i(S(t)+p(t)\cdot(x-q(t)))/\varepsilon},$$

where (q,p) is given by (1.3), S is the classical action (1.4), and the envelope u solves the nonlinear equation

$$i\partial_t u + \frac{1}{2}\Delta u = \frac{1}{2}\left\langle y, \nabla^2 V\left(t, q(t)\right) y\right\rangle u + \lambda\left(|y|^{-\gamma} * |u|^2\right) u.$$

It is proved that two such wave packets evolve independently from each other, up to an error which is $\mathcal{O}\left(\varepsilon^{\frac{\gamma}{2(1+\gamma)}}\right)$. A way to understand this result compared to the ones presented here is that since $\alpha_c > 1$, no interference can occur at leading order.

There are several results which may seem similar to ours, in the case of one initial wave packet: see e.g. [7, 16, 19, 27, 28, 29, 30]. In those papers, the initial amplitude a is very specific, since it is a ground state. The propagation and stability of multi-solitons for the nonlinear Schrödinger equation (without external potential) have been studied in [33, 34, 35, 37] (see also [40]). In the framework of these papers, the waves do not interfere.

In [1], a problem which shares several features with ours is studied: there is an external potential, the regime is semiclassical (see [27]), and nonlinear. The envelopes of the initial data are two solitons. The structure of the soliton manifold implies some rigidity on the evolution of the initial data. Eventually, the two waves do not interact at leading order.

On the other hand, in [31], the case of two solitons for the Hartree equation has been studied. In this non-semiclassical setting, and in the absence of an external potential, the authors construct a solution which behaves, for large time, like the sum of two solitary waves, whose respective centers in phase space evolve according to the two-body problem. This feature can be compared to Theorem 1.9 (with $V = 0$), where the centers of the wave packets evolve according to the nonlinear system (1.12). Nevertheless, the envelopes are given by the ground state, and do not evolve with time. The analytical approach is different: in [31], a fine study of the Hartree operator linearized about the soliton is performed, in particular to understand the spectral properties of this operator. On the other hand, we do not consider such an operator; a similar approach with general profiles a_1, a_2 like we consider would probably be out of reach.

In [23, 38, 39], a semiclassical regime is studied, in the presence of an external potential and a nonlinearity. The potential is a double well potential, and the associated Hamiltonian has two eigenfunctions. For initial data carried by these two eigenfunctions, it is shown that the nonlinear solution may remain concentrated on the eigenfunctions, with time-dependent coefficients which interact nonlinearly.

In all the cases mentioned above, the nonlinear interference of the envelopes is negligible, due to the fact that the envelopes decay exponentially. In our case, the decay may be much weaker (algebraic). However, even though we have seen that the envelopes always interact nonlinearly in the cases studied here, we will see that some "rectangle" terms are negligible in the limit $\varepsilon \to 0$, thanks to a microlocal argument (see Section 3).

We finally point out that nonlinear interactions of amplitudes have been analyzed in the context of weakly nonlinear geometric optics for Schrödinger or Hartree equations in various contexts (not to mention the even wider literature concerning hyperbolic equations); see for instance [11, 22].

Notations. Throughout this paper, $\mathbf{R}_+$ stands for $[0,\infty)$. We also use the standard convention, for $A \in \mathbf{R}^n$, $n \geqslant 1$,

$$\langle A \rangle = \sqrt{1+|A|^2}.$$

For two positive numbers a^ε and b^ε, the notation $a^\varepsilon \lesssim b^\varepsilon$ means that there exists $C>0$ *independent of* ε such that for all $\varepsilon \in (0,1]$, $a^\varepsilon \leqslant C b^\varepsilon$.

2. Formal derivation

We resume the same approach as in the case of a single wave packet ([9]), in the case of (1.6): from this point of view the computations below include the ones presented in [9].

2.1. **The general strategy.**

We seek an approximate solution of the form

$$\psi^\varepsilon_{\rm app}(t,x) = \varepsilon^{-d/4} \sum_{j=1,2} u_j\left(t, \frac{x-q_j(t)}{\sqrt{\varepsilon}}\right) e^{i(S_j(t)+p_j(t)\cdot(x-q_j(t)))/\varepsilon}, \tag{2.1}$$

for some profiles u_j independent of ε, and some functions $S_j(t)$ to be determined. These functions S_j correspond to the classical action (1.4) in the linear case. We will see that according to the value α in (1.1), the expression of S_j may vary, accounting for nonlinear effects due to the presence of the Hartree nonlinearity, and so it may be convenient to consider ε-dependent functions S_j. Also, according to the value of α, the pairs (q_j,p_j) will solve the standard Hamiltonian system (1.3), or a modified one. Denote

$$\phi_j(t,x) = S_j(t) + p_j(t)\cdot(x-q_j(t)).$$

In the cases $\alpha = 0, 1/2$ and $\alpha = 1$ considered in this paper, we will see that we can write

$$\begin{aligned} &i\varepsilon\partial_t \psi^\varepsilon_{\rm app} + \frac{\varepsilon^2}{2}\Delta \psi^\varepsilon_{\rm app} - V\psi^\varepsilon_{\rm app} - \varepsilon^\alpha\left(K * |\psi^\varepsilon_{\rm app}|^2\right)\psi^\varepsilon_{\rm app} = \\ &\quad \varepsilon^{-d/4}\sum_{j=1,2} e^{i\phi_j(t,x)/\varepsilon}\left(b_{0j} + \sqrt{\varepsilon} b_{1j} + \varepsilon b_{2j} + \varepsilon r_j^\varepsilon\right)\left(t, \frac{x-q_j(t)}{\sqrt{\varepsilon}}\right), \end{aligned} \tag{2.2}$$

for b_{ij} independent of ε. The approximate solution $\psi^\varepsilon_{\rm app}$ is determined by the conditions

$$b_{0j} = b_{1j} = b_{2j} = 0, \quad j=1,2.$$

The remaining factor r_j^ε accounts for the error between the exact solution ψ^ε and the approximate solution $\psi^\varepsilon_{\rm app}$. Introduce two new space variables, which are naturally associated to each of the two approximating wave packets:

$$y_j = \frac{x-q_j(t)}{\sqrt{\varepsilon}}, \quad j=1,2.$$

At this stage, the introduction of these variables may seem very artificial, since only the x variable will eventually remain. It can be understood as a change of variable corresponding to the moving frame of each wave packet. Technically, it will be justified by the fact, already present in the linear case $K=0$, that the remainders r_j^ε will satisfy pointwise estimates of the form

$$\left| r_j^\varepsilon\left(t, \frac{x-q_j(t)}{\sqrt{\varepsilon}}\right)\right| \lesssim \sqrt{\varepsilon}\left\langle y_j\right\rangle^3 A_j^\varepsilon(t,y_j)\Big|_{y_j = \frac{x-q_j(t)}{\sqrt{\varepsilon}}}.$$

The functions A_j^ε are well localized, in the sense that $y_j \mapsto \left\langle y_j\right\rangle^k A_j^\varepsilon(t,y_j)$ in bounded in $L^2(\mathbf{R}^d)$ at least for $k=3$ (but possibly for larger k's), while typically, a function of the

form

$$\left\langle y_j + \eta \frac{q_1(t) - q_2(t)}{\sqrt{\varepsilon}} \right\rangle^3 A_j^\varepsilon(t, y_j)$$

cannot be controlled in $L^2(\mathbf{R}^d)$ uniformly in ε and $t \in [0, T]$ if $\eta \neq 0$.

To conclude this subsection, we expand each term on the left hand side of (2.2) so it has the form of the right hand side. In the following subsections, we discuss the outcome according to the value $\alpha = 0, 1/2$ or $\alpha = 1$.

The linear terms are computed as follows:

$$i\varepsilon\partial_t\psi^\varepsilon_{\rm app} = \varepsilon^{-d/4} \sum_{j=1,2} e^{i\phi_j(t,x)/\varepsilon} \left(i\varepsilon\partial_t u_j - i\sqrt{\varepsilon}\dot{q}_j(t)\cdot\nabla u_j - u_j\partial_t\phi_j\right).$$

$$\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon_{\rm app} = \varepsilon^{-d/4} \sum_{j=1,2} e^{i\phi_j(t,x)/\varepsilon} \left(\frac{\varepsilon}{2}\Delta u_j + i\sqrt{\varepsilon}p_j(t)\cdot\nabla u_j - \frac{|p_j(t)|^2}{2}u_j\right).$$

Here, as well as below, one should remember that the functions are assessed as in (2.1). Recalling that the relevant space variable for u_j is y_j, we have:

$$\partial_t\phi_j = \dot{S}_j(t) + \frac{d}{dt}\left(p_j(t)\cdot(x - q_j(t))\right) = \dot{S}_j(t) + \sqrt{\varepsilon}\dot{p}_j(t)\cdot y_j - p_j(t)\cdot\dot{q}_j(t).$$

For the linear potential term, we write

$$\begin{aligned} V\psi^\varepsilon_{\rm app} &= V(t,x)\varepsilon^{-d/4}\sum_{j=1,2} e^{i\phi_j(t,x)/\varepsilon} u_j\left(t, y_j\right) \\ &= \varepsilon^{-d/4}\sum_{j=1,2} e^{i\phi_j(t,x)/\varepsilon} V\left(t, q_j(t) + y_j\sqrt{\varepsilon}\right) u_j\left(t, y_j\right), \end{aligned}$$

and we perform a Taylor expansion for V about $x = q_j(t)$:

$$\begin{aligned} V\left(t, q_j(t) + y_j\sqrt{\varepsilon}\right) u_j(t, y_j) &= V\left(t, q_j(t)\right) u_j(t, y_j) + \sqrt{\varepsilon} y_j\cdot\nabla V\left(t, q_j(t)\right) u_j(t, y_j) \\ &\quad + \frac{\varepsilon}{2}\left\langle y_j, \nabla^2 V\left(t, q_j(t)\right) y_j\right\rangle u_j(t, y_j) + \varepsilon^{3/2} r^\varepsilon_{jV}(t, y_j), \end{aligned}$$

with

$$|r^\varepsilon_{jV}(t, y_j)| \leqslant C\left\langle y_j\right\rangle^3 |u_j(t, y_j)|, \tag{2.3}$$

for some C independent of ε, t and y_j, in view of Assumption 1.1. In the case $K = 0$, we come up with the relations:

$$\begin{aligned} b^{\rm lin}_{0j} &= -u_j\left(\dot{S}_j(t) - p_j(t)\cdot\dot{q}_j(t) + \frac{|p_j(t)|^2}{2} + V\left(t, q_j(t)\right)\right). \\ b^{\rm lin}_{1j} &= -i\left(\dot{q}_j(t) - p_j(t)\right)\cdot\nabla u_j - y_j\cdot\left(\dot{p}_j(t) + \nabla V\left(t, q_j(t)\right)\right) u_j. \\ b^{\rm lin}_{2j} &= i\partial_t u_j + \frac{1}{2}\Delta u_j - \frac{1}{2}\left\langle y_j, \nabla^2 V\left(t, q_j(t)\right) y_j\right\rangle u_j. \end{aligned}$$

For the nonlinear term, the computations are heavier:

$$\left(K * |\psi^\varepsilon_{\rm app}|^2\right)\psi^\varepsilon_{\rm app} = \varepsilon^{-d/4}\sum_{j=1,2} e^{i\phi_j(t,x)/\varepsilon}\left(\int K(z)|\psi^\varepsilon_{\rm app}(t, x - z)|^2 dz\right) u_j(t, y_j).$$

Eventually, each envelope u_j will solve a Schrödinger equation, the two equations being coupled. The precise expression of these equations depends on α, but at this stage, we can

notice that for $j=1,2$, u_j solves an equation of the form

$$i\partial_t u_j + \frac{1}{2}\Delta u_j = \frac{1}{2}\left\langle y_j, \nabla^2 V\left(t,q_j(t)\right) y_j\right\rangle u_j + F_j u_j, \tag{2.4}$$

where the function F_j, accounting for nonlinear effects due to the Hartree kernel, is *real-valued*. We infer an important property: the L^2-norm of u_j is independent of time,

$$\|u_j(t)\|_{L^2(\mathbf{R}^d)} = \|a_j\|_{L^2(\mathbf{R}^d)}, \quad \forall t\geqslant 0,\ j=1,2. \tag{2.5}$$

At this stage, this is only a formal remark.

In the above sum, the variable x must be expressed in terms of y_j:

$$\begin{aligned}
K*|\psi^\varepsilon_{\rm app}|^2 &= \int K(z)\left|\psi^\varepsilon_{\rm app}\left(t,q_j(t)+\sqrt{\varepsilon}y_j - z\right)\right|^2 dz\\
&= \varepsilon^{-d/2}\int K(z)\left|\sum_{k=1,2} e^{i\phi_k(t,x-z)/\varepsilon}u_k\left(t,y_j+\frac{q_j(t)-q_k(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2 dz.
\end{aligned}$$

Before changing the integration variable, we develop the squared modulus:

$$\begin{aligned}
&\left|\sum_{k=1,2} e^{i\phi_k(t,x-z)/\varepsilon}u_k\left(t,y_j+\frac{q_j(t)-q_k(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2 =\\
&\left|u_1\left(t,y_j+\frac{q_j(t)-q_1(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2 + \left|u_2\left(t,y_j+\frac{q_j(t)-q_2(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2\\
&+2\,\mathrm{Re}\, e^{i(\phi_1-\phi_2)/\varepsilon}u_1\left(t,y_j+\frac{q_j(t)-q_1(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\overline{u}_2\left(t,y_j+\frac{q_j(t)-q_2(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right),
\end{aligned}$$

where $\phi_1-\phi_2$ stands for $\phi_1(t,x-z)-\phi_2(t,x-z)$. To ease notations, we shall denote in the rest of this paper:

$$\delta q(t) = q_1(t)-q_2(t);\quad \delta p(t) = p_1(t)-p_2(t).$$

We can write

$$\left(K*|\psi^\varepsilon_{\rm app}|^2\right)\psi^\varepsilon_{\rm app} = \varepsilon^{-d/4}\sum_{j=1,2} e^{i\phi_j(t,x)/\varepsilon}V_j^{\rm NL}(t,y_j)u_j(t,y_j),$$

with

$$\begin{aligned}
V_1^{\rm NL}(t,y_1) &= \varepsilon^{-d/2}\int K(z)\Bigg(\left|u_1\left(t,y_1-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2+\left|u_2\left(t,y_1+\frac{\delta q(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2\\
&\qquad + 2\,\mathrm{Re}\, e^{i(\phi_1-\phi_2)/\varepsilon}u_1\left(t,y_1-\frac{z}{\sqrt{\varepsilon}}\right)\overline{u}_2\left(t,y_1+\frac{\delta q(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\Bigg)dz,\\
V_2^{\rm NL}(t,y_2) &= \varepsilon^{-d/2}\int K(z)\Bigg(\left|u_1\left(t,y_2-\frac{\delta q(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2+\left|u_2\left(t,y_2-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2\\
&\qquad + 2\,\mathrm{Re}\, e^{i(\phi_1-\phi_2)/\varepsilon}u_1\left(t,y_2-\frac{\delta q(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\overline{u}_2\left(t,y_2-\frac{z}{\sqrt{\varepsilon}}\right)\Bigg)dz.
\end{aligned}$$

Each nonlinear potential $V_j^{\rm NL}$ is the sum of three terms. The third term in each of these two expressions, involving the product $u_1\overline{u}_2$, will be referred to as *rectangle term*, as opposed to *squared terms*, involving squared moduli. The two rectangle terms are examined in Section 3, where we show that at least on finite time intervals, they are negligible in the

limit $\varepsilon \to 0$, regardless of the value of α. Therefore, we now consider only the squared terms. Changing variables in the integrations and performing a Taylor expansion of the kernel K, we find successively (recall that G_j is defined by (1.14)):

$$\begin{aligned}\varepsilon^{-d/2}\int K(z)\left|u_1\left(t,y_1-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2 dz &= \int K\left(\sqrt{\varepsilon}(y_1-z)\right)\left|u_1\left(t,z\right)\right|^2 dz\\ &= K(0)\|a_1\|^2_{L^2}+\sqrt{\varepsilon}\|a_1\|^2_{L^2}y_1\cdot\nabla K(0)-\sqrt{\varepsilon}\nabla K(0)\cdot G_1(t)\\ &+\frac{\varepsilon}{2}\left\langle y_1,\nabla^2K(0)y_1\right\rangle\|a_1\|^2_{L^2}+\frac{\varepsilon}{2}\int\left\langle z,\nabla^2K(0)z\right\rangle|u_1(t,z)|^2dz\\ &-\varepsilon\left\langle\nabla^2K(0)G_1(t),y_1\right\rangle+\varepsilon^{3/2}\int r^{\varepsilon}_{11}(t,z-y_1)|u_1(t,z)|^2dz,\end{aligned}$$

$$\begin{aligned}\varepsilon^{-d/2}\int K(z)&\left|u_2\left(t,y_1+\frac{\delta q(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2 dz\\ &= \int K\left(\delta q(t)+\sqrt{\varepsilon}(y_1-z)\right)\left|u_2\left(t,z\right)\right|^2 dz\\ &= K(\delta q)\|a_2\|^2_{L^2}+\sqrt{\varepsilon}\|a_2\|^2_{L^2}y_1\cdot\nabla K(\delta q)-\sqrt{\varepsilon}\nabla K(\delta q)\cdot G_2(t)\\ &+\frac{\varepsilon}{2}\left\langle y_1,\nabla^2K(\delta q)y_1\right\rangle\|a_2\|^2_{L^2}+\frac{\varepsilon}{2}\int\left\langle z,\nabla^2K(\delta q)z\right\rangle|u_2(t,z)|^2dz\\ &-\varepsilon\left\langle\nabla^2K(\delta q)G_2(t),y_1\right\rangle+\varepsilon^{3/2}\int r^{\varepsilon}_{12}(t,z-y_1)|u_2(t,z)|^2dz,\end{aligned}$$

$$\begin{aligned}\varepsilon^{-d/2}\int K(z)&\left|u_1\left(t,y_2-\frac{\delta q(t)}{\sqrt{\varepsilon}}-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2 dz\\ &= K(-\delta q)\|a_1\|^2_{L^2}+\sqrt{\varepsilon}\|a_1\|^2_{L^2}y_2\cdot\nabla K(-\delta q)-\sqrt{\varepsilon}\nabla K(-\delta q)\cdot G_1(t)\\ &+\frac{\varepsilon}{2}\left\langle y_2,\nabla^2K(-\delta q)y_2\right\rangle\|a_1\|^2_{L^2}+\frac{\varepsilon}{2}\int\left\langle z,\nabla^2K(-\delta q)z\right\rangle|u_1(t,z)|^2dz\\ &-\varepsilon\left\langle\nabla^2K(-\delta q)G_1(t),y_2\right\rangle+\varepsilon^{3/2}\int r^{\varepsilon}_{21}(t,z-y_2)|u_1(t,z)|^2dz,\end{aligned}$$

$$\begin{aligned}\varepsilon^{-d/2}\int K(z)&\left|u_2\left(t,y_2-\frac{z}{\sqrt{\varepsilon}}\right)\right|^2 dz\\ &= K(0)\|a_2\|^2_{L^2}+\sqrt{\varepsilon}\|a_2\|^2_{L^2}y_2\cdot\nabla K(0)-\sqrt{\varepsilon}\nabla K(0)\cdot G_2(t)\\ &+\frac{\varepsilon}{2}\left\langle y_2,\nabla^2K(0)y_2\right\rangle\|a_2\|^2_{L^2}+\frac{\varepsilon}{2}\int\left\langle z,\nabla^2K(0)z\right\rangle|u_2(t,z)|^2dz\\ &-\varepsilon\left\langle\nabla^2K(0)G_2(t),y_2\right\rangle+\varepsilon^{3/2}\int r^{\varepsilon}_{22}(t,z-y_2)|u_2(t,z)|^2dz,\end{aligned}$$

where the functions r^{ε}_{jk} satisfy uniform estimates of the form

$$|r^{\varepsilon}_{jk}(t,z)|\leqslant C(T)\left\langle z\right\rangle^3,\quad\forall z\in\mathbf{R}^d,t\in[0,T],\tag{2.6}$$

with $C(T)$ independent of ε, j and k, but possibly depending on T.

2.2. **The critical case:** $\alpha = 1$**.** When $\alpha > 1$, we have $b_{\ell j} = b_{\ell j}^{\rm lin}$ for all ℓ, j: nonlinear effects are not present at leading order. When $\alpha = 1$, we still have $b_{\ell j} = b_{\ell j}^{\rm lin}$ for $\ell = 0, 1$: we still demand (q_j, p_j) to solve (1.3) in order for the equations $b_{\ell j} = 0$, $\ell = 0, 1$, to be satisfied, and S_j is defined as in (1.4). On the other hand, the expression for b_{2j} is altered:

$$\begin{aligned} b_{21} &= i\partial_t u_1 + \frac{1}{2}\Delta u_1 - \frac{1}{2}\left\langle y_1, \nabla^2 V\left(t, q_1(t)\right) y_1\right\rangle u_1 - K(0)\|a_1\|_{L^2}^2 u_1 \\ &\quad - K\left(\delta q(t)\right)\|a_2\|_{L^2}^2 u_1, \\ b_{22} &= i\partial_t u_2 + \frac{1}{2}\Delta u_2 - \frac{1}{2}\left\langle y_2, \nabla^2 V\left(t, q_2(t)\right) y_2\right\rangle u_2 - K(0)\|a_2\|_{L^2}^2 u_2 \\ &\quad - K\left(-\delta q(t)\right)\|a_1\|_{L^2}^2 u_2. \end{aligned}$$

The last term in each expression accounts for a coupling, revealing a leading order interaction of the two wave packets. This coupling can be understood rather explicitly, since it consists of a purely time dependent potential. Solving the equations $b_{2j} = 0$, we infer, with obvious notations adapted from (1.5),

$$\begin{aligned} u_1(t, y_1) &= u_1^{\rm lin}(t, y_1) \exp\left(-itK(0)\|a_1\|_{L^2}^2 - i\|a_2\|_{L^2}^2 \int_0^t K\left(\delta q(s)\right) ds\right), \\ u_2(t, y_2) &= u_2^{\rm lin}(t, y_2) \exp\left(-itK(0)\|a_2\|_{L^2}^2 - i\|a_1\|_{L^2}^2 \int_0^t K\left(-\delta q(s)\right) ds\right). \end{aligned}$$

The presence of these phase shifts accounts for nonlinear effects at leading order in the approximate wave packet $\psi^\varepsilon_{\rm app}$: nonlinear effects in the case of a single wave packet, and nonlinear coupling, since we assume $\|a_j\|_{L^2} \neq 0$. For the remainder terms, we have the (rough) pointwise estimate

$$|r_j^\varepsilon(t, y_j)| \leqslant C(T)\sqrt{\varepsilon}\left\langle y_j\right\rangle^3 |u_j(t, y_j)| \left(1 + \sum_{k=1,2} \|u_k(t)\|_{\Sigma^2}^2\right), \quad t \in [0, T]. \tag{2.7}$$

The remainder r_j^ε is the sum of the terms r_{jV}^ε and $\varepsilon^{\alpha+3/2}(r_{jk}^\varepsilon * |u_k|^2)u_j$, $k = 1, 2$, so this estimate is an easy consequence of (2.3) and (2.6). To be precise, this estimate is valid up to the rectangle terms that we have discarded so far, when we have developed $(K * |\psi^\varepsilon_{\rm app}|^2)\psi^\varepsilon_{\rm app}$. We will see in Section 3 that they satisfy a similar estimate (see Corollary 3.2).

2.3. **The case** $\alpha = 1/2$**.** We still have $b_{0j} = b_{0j}^{\rm lin}$, but now

$$\begin{aligned} b_{11} &= -i\left(\dot q_1(t) - p_1(t)\right)\cdot\nabla u_1 - y_1\cdot\left(\dot p_1(t) + \nabla V\left(t, q_1(t)\right)\right) u_1 \\ &\quad - K(0)\|a_1\|_{L^2}^2 u_1 - K\left(\delta q\right)\|a_2\|_{L^2}^2 u_1, \\ b_{12} &= -i\left(\dot q_2(t) - p_2(t)\right)\cdot\nabla u_2 - y_2\cdot\left(\dot p_2(t) + \nabla V\left(t, q_2(t)\right)\right) u_2 \\ &\quad - K(0)\|a_2\|_{L^2}^2 u_2 - K\left(-\delta q\right)\|a_1\|_{L^2}^2 u_2, \\ b_{21} &= i\partial_t u_1 + \frac{1}{2}\Delta u_1 - \frac{1}{2}\left\langle y_1, \nabla^2 V\left(t, q_1(t)\right) y_1\right\rangle u_1 - \|a_1\|_{L^2}^2 y_1\cdot\nabla K(0) u_1 \\ &\quad - \|a_2\|_{L^2}^2 y_1\cdot\nabla K(\delta q) u_1 + \nabla K(0)\cdot G_1(t) u_1 + \nabla K(\delta q)\cdot G_2(t) u_1, \\ b_{22} &= i\partial_t u_2 + \frac{1}{2}\Delta u_2 - \frac{1}{2}\left\langle y_2, \nabla^2 V\left(t, q_2(t)\right) y_2\right\rangle u_2 - \|a_2\|_{L^2}^2 y_2\cdot\nabla K(0) u_2 \\ &\quad - \|a_1\|_{L^2}^2 y_2\cdot\nabla K(-\delta q) u_2 + \nabla K(0)\cdot G_2(t) u_2 + \nabla K(-\delta q)\cdot G_1(t) u_2. \end{aligned}$$

The first line in b_{1j} is zero if (q_j, p_j) is the classical trajectory given by (1.3). On the other hand, it does not seem to be possible to cancel out the second line in b_{1j}, even by modifying (1.3): we have three sets of terms, involving ∇u_1, $y_1 u_1$ and u_1, respectively, so they must be treated separately. As in [9], we then modify the general strategy, and allow b_{0j} to depend on ε. We alter the hierarchy as follows:

$$\begin{aligned}
b_{01}^\varepsilon &= -u_1\Big(\dot{S}_1(t) - p_1(t)\cdot\dot{q}_1(t) + \frac{|p_1(t)|^2}{2} + V\left(t, q_1(t)\right)\\
&\qquad + \sqrt{\varepsilon}K(0)\|a_1\|_{L^2}^2 + \sqrt{\varepsilon}K\left(\delta q\right)\|a_2\|_{L^2}^2\Big),\\
b_{02}^\varepsilon &= -u_2\Big(\dot{S}_2(t) - p_2(t)\cdot\dot{q}_2(t) + \frac{|p_2(t)|^2}{2} + V\left(t, q_2(t)\right)\\
&\qquad + \sqrt{\varepsilon}K(0)\|a_2\|_{L^2}^2 + \sqrt{\varepsilon}K\left(-\delta q\right)\|a_1\|_{L^2}^2\Big),\\
b_{11} &= -i\left(\dot{q}_1(t) - p_1(t)\right)\cdot\nabla u_1 - y_1\cdot\left(\dot{p}_1(t) + \nabla V\left(t, q_1(t)\right)\right)u_1,\\
b_{12} &= -i\left(\dot{q}_2(t) - p_2(t)\right)\cdot\nabla u_2 - y_2\cdot\left(\dot{p}_2(t) + \nabla V\left(t, q_2(t)\right)\right)u_2,
\end{aligned}$$

and we leave b_{2j} unchanged. Like before, $b_{1j}=0$ provided that (q_j, p_j) solves (1.3). The novelty is that we now consider modified, ε-dependent, actions:

$$\begin{cases}
S_1^\varepsilon(t) = \displaystyle\int_0^t \left(\frac{1}{2}|p_1(s)|^2 - V(s, q_1(s))\right)ds\\
\qquad\qquad - t\sqrt{\varepsilon}K(0)\|a_1\|_{L^2(\mathbf{R}^d)}^2 - \sqrt{\varepsilon}\|a_2\|_{L^2(\mathbf{R}^d)}^2 \displaystyle\int_0^t K\left(\delta q(s)\right)ds,\\
S_2^\varepsilon(t) = \displaystyle\int_0^t \left(\frac{1}{2}|p_2(s)|^2 - V(s, q_2(s))\right)ds\\
\qquad\qquad - t\sqrt{\varepsilon}K(0)\|a_2\|_{L^2(\mathbf{R}^d)}^2 - \sqrt{\varepsilon}\|a_1\|_{L^2(\mathbf{R}^d)}^2 \displaystyle\int_0^t K\left(-\delta q(s)\right)ds.
\end{cases}$$

These expressions are exactly those given in the introduction (1.9). The equations $b_{2j}=0$ are envelope equations, which are nonlinear since G_k is a nonlinear function of u_k. Note however that G_k yields a purely time-dependent potential. Consider the solution to

$$\begin{aligned}
i\partial_t\tilde{u}_1 + \frac{1}{2}\Delta\tilde{u}_1 &= \frac{1}{2}\left\langle y_1, \nabla^2 V\left(t, q_1(t)\right)y_1\right\rangle\tilde{u}_1 + \|a_1\|_{L^2}^2 y_1\cdot\nabla K(0)\tilde{u}_1\\
&\quad + \|a_2\|_{L^2}^2 y_1\cdot\nabla K(\delta q)\tilde{u}_1,\\
i\partial_t\tilde{u}_2 + \frac{1}{2}\Delta\tilde{u}_2 &= \frac{1}{2}\left\langle y_2, \nabla^2 V\left(t, q_2(t)\right)y_2\right\rangle\tilde{u}_2 + \|a_2\|_{L^2}^2 y_2\cdot\nabla K(0)\tilde{u}_2\\
&\quad + \|a_1\|_{L^2}^2 y_2\cdot\nabla K(-\delta q)\tilde{u}_2.
\end{aligned}$$

Set

$$\begin{aligned}
u_1(t, y_1) &= \tilde{u}_1(t, y_1)\exp\left(i\int_0^t\Big(\nabla K(0)\cdot\tilde{G}_1(s) + \nabla K\left(\delta q(s)\right)\cdot\tilde{G}_2(s)\Big)ds\right),\\
u_2(t, y_2) &= \tilde{u}_2(t, y_2)\exp\left(i\int_0^t\Big(\nabla K(0)\cdot\tilde{G}_2(s) + \nabla K\left(-\delta q(s)\right)\cdot\tilde{G}_1(s)\Big)ds\right),
\end{aligned}$$

where

$$\tilde{G}_j(t) = \int_{\mathbf{R}^d} z|\tilde{u}_j(t,z)|^2 dz.$$

It is clear that $|u_j| = |\tilde{u}_j|$, hence $\tilde{G}_j = G_j$, and so u_1 and u_2 are such that $b_{21} = b_{22} = 0$, and correspond to the envelopes introduced in §1.4. Finally, we still have a remainder term satisfying (2.7) (up to the terms treated in §3).

2.4. **The case $\alpha = 0$.** Now all the coefficients $b_{\ell j}$ are affected by the nonlinearity:

$$\begin{aligned}
b_{01} &= -u_1\Big(\dot{S}_1(t) - p_1(t)\cdot \dot{q}_1(t) + \frac{|p_1(t)|^2}{2} + V\left(t,q_1(t)\right) + K(0)\|a_1\|^2_{L^2}\\
&\qquad\qquad + K\left(\delta q\right)\|a_2\|^2_{L^2}\Big),\\
b_{02} &= -u_2\Big(\dot{S}_2(t) - p_2(t)\cdot \dot{q}_2(t) + \frac{|p_2(t)|^2}{2} + V\left(t,q_2(t)\right) + K(0)\|a_2\|^2_{L^2}\\
&\qquad\qquad + K\left(-\delta q\right)\|a_1\|^2_{L^2}\Big),\\
b_{11} &= -i\left(\dot{q}_1(t) - p_1(t)\right)\cdot\nabla u_1 - y_1\cdot\left(\dot{p}_1(t) + \nabla V\left(t,q_1(t)\right)\right)u_1 - \|a_1\|^2_{L^2} y_1\cdot\nabla K(0) u_1\\
&\quad - \|a_2\|^2_{L^2} y_1\cdot \nabla K\left(\delta q\right)u_1 + \nabla K(0)\cdot G_1(t) u_1 + \nabla K\left(\delta q\right)\cdot G_2(t) u_1,\\
b_{12} &= -i\left(\dot{q}_2(t) - p_2(t)\right)\cdot\nabla u_2 - y_2\cdot\left(\dot{p}_2(t) + \nabla V\left(t,q_2(t)\right)\right)u_2 - \|a_2\|^2_{L^2} y_2\cdot\nabla K(0) u_2\\
&\quad - \|a_1\|^2_{L^2} y_2\cdot \nabla K\left(-\delta q\right)u_2 + \nabla K(0)\cdot G_2(t) u_2 + \nabla K\left(-\delta q\right)\cdot G_1(t) u_2,\\
b_{21} &= i\partial_t u_1 + \frac{1}{2}\Delta u_1 - \frac{1}{2}\left\langle y_1, M_1(t) y_1\right\rangle u_1 + \left\langle \nabla^2 K(0) G_1(t), y_1\right\rangle u_1\\
&\quad + \left\langle \nabla^2 K(\delta q) G_2(t), y_1\right\rangle u_1 - \frac{1}{2}\left(\int \left\langle z, \nabla^2 K(0) z\right\rangle |u_1(t,z)|^2 dz\right) u_1\\
&\quad - \frac{1}{2}\left(\int \left\langle z, \nabla^2 K(\delta q) z\right\rangle |u_2(t,z)|^2 dz\right) u_1,\\
b_{22} &= i\partial_t u_2 + \frac{1}{2}\Delta u_2 - \frac{1}{2}\left\langle y_2, M_2(t) y_2\right\rangle u_2 + \left\langle \nabla^2 K(0) G_2(t), y_2\right\rangle u_2\\
&\quad + \left\langle \nabla^2 K(-\delta q) G_1(t), y_2\right\rangle u_2 - \frac{1}{2}\left(\int \left\langle z, \nabla^2 K(0) z\right\rangle |u_2(t,z)|^2 dz\right) u_2\\
&\quad - \frac{1}{2}\left(\int \left\langle z, \nabla^2 K(-\delta q) z\right\rangle |u_1(t,z)|^2 dz\right) u_2,
\end{aligned}$$

where we have denoted

$$\begin{aligned}
M_1(t) &= \|a_1\|^2_{L^2(\mathbf{R}^d)}\nabla^2 K(0) + \|a_2\|^2_{L^2(\mathbf{R}^d)}\nabla^2 K\left(\delta q(t)\right) + \nabla^2_x V\left(t,q_1(t)\right),\\
M_2(t) &= \|a_2\|^2_{L^2(\mathbf{R}^d)}\nabla^2 K(0) + \|a_1\|^2_{L^2(\mathbf{R}^d)}\nabla^2 K\left(-\delta q(t)\right) + \nabla^2_x V\left(t,q_2(t)\right).
\end{aligned}$$

Similar to the case $\alpha = 1/2$, we incorporate the last term of b_{1j} into b_{0j}, that is we modify the action as follows:

$$\begin{aligned}
S_1^\varepsilon(t) = \int_0^t \Big(&\frac{1}{2}|p_1(s)|^2 - V\left(s,q_1(s)\right) - K(0)\|a_1\|^2_{L^2} - K\left(\delta q(s)\right)\|a_2\|^2_{L^2}\\
&+ \sqrt{\varepsilon}\nabla K(0)\cdot G_1(s) + \sqrt{\varepsilon}\nabla K\left(\delta q(s)\right)\cdot G_2(s)\Big) ds,\\
S_2^\varepsilon(t) = \int_0^t \Big(&\frac{1}{2}|p_2(s)|^2 - V\left(s,q_2(s)\right) - K(0)\|a_2\|^2_{L^2} - K\left(-\delta q(s)\right)\|a_1\|^2_{L^2}\\
&+ \sqrt{\varepsilon}\nabla K(0)\cdot G_2(s) + \sqrt{\varepsilon}\nabla K\left(-\delta q(s)\right)\cdot G_1(s)\Big) ds.
\end{aligned}$$

Note that for S_j^ε to be well defined, we have to first define u_j, for which we solve the envelope equations, given by $b_{21} = b_{22} = 0$. Canceling the terms b_{1j} yields the modified system of trajectories:

$$\begin{cases} \dot{q}_1(t) = p_1(t), \\ \dot{p}_1(t) = -\nabla V\left(t, q_1(t)\right) - \|a_1\|_{L^2}^2 \nabla K(0) - \|a_2\|_{L^2}^2 \nabla K\left(q_1(t) - q_2(t)\right), \\ \dot{q}_2(t) = p_2(t), \\ \dot{p}_2(t) = -\nabla V\left(t, q_2(t)\right) - \|a_2\|_{L^2}^2 \nabla K(0) - \|a_1\|_{L^2}^2 \nabla K\left(q_2(t) - q_1(t)\right), \end{cases}$$

which is exactly (1.12). The remainder term still satisfies (2.7) (up to the terms treated in §3). We will examine more carefully the envelope system in §5.

3. Analysis of the rectangle interaction term

In the previous section, we have left out the rectangle terms, claiming that they are negligible in the limit $\varepsilon \to 0$. In this section, we justify precisely this statement. Since the two terms that we have discarded are similar, we shall simply consider the first one:

$$2\varepsilon^{-d/2} \operatorname{Re} \int K(z) e^{i(\phi_1 - \phi_2)(t, x-z)/\varepsilon} u_1\left(t, y_1 - \frac{z}{\sqrt{\varepsilon}}\right) \overline{u}_2\left(t, y_1 + \frac{\delta q(t)}{\sqrt{\varepsilon}} - \frac{z}{\sqrt{\varepsilon}}\right) dz.$$

Notice that we have not yet expressed the phases ϕ_k in terms of the variable y_1, and that the expression of ϕ_k varies according to $\alpha = 1$, $\alpha = 1/2$, or $\alpha = 0$. We shall retain only a common feature though, that is, $\phi_k^\varepsilon(t, x) = \Theta_k^\varepsilon(t) + x \cdot p_k(t)$, where only the purely time dependent function Θ may depend on ε (when $\alpha \in \{1/2, 0\}$), and the spatial oscillations are singled out. Since $x = q_1(t) + \sqrt{\varepsilon} y_1$, we get, once the real part and the time oscillations are omitted:

$$\varepsilon^{-d/2} \int K(z) e^{i\left(\sqrt{\varepsilon} y_1 - z\right) \cdot \delta p(t)/\varepsilon} u_1\left(t, y_1 - \frac{z}{\sqrt{\varepsilon}}\right) \overline{u}_2\left(t, y_1 + \frac{\delta q(t)}{\sqrt{\varepsilon}} - \frac{z}{\sqrt{\varepsilon}}\right) dz.$$

Changing the integration variable, and introducing more general notations, we examine:

$$I^\varepsilon(t, y_1) = \int \mathcal{K}\left(\sqrt{\varepsilon}(y_1 - z)\right) e^{iz \cdot \delta p(t)/\sqrt{\varepsilon}} u_1\left(t, z\right) \overline{u}_2\left(t, z + \frac{\delta q(t)}{\sqrt{\varepsilon}}\right) dz. \tag{3.1}$$

The main result of this section is stated as follows.

Proposition 3.1. *Let $T > 0$. Suppose that $\mathcal{K} \in W^{\ell,\infty}$, $u_j \in C([0, T]; \Sigma^k)$ with $k, \ell \in \mathbf{N}$, and consider I^ε defined by* (3.1)*. There exists $C > 0$ independent of $\varepsilon \in (0, 1]$, $\mathcal{K}$, u_1 and u_2 such that*

$$\sup_{t \in [0,T]} \|I^\varepsilon(t, \cdot)\|_{L^\infty(\mathbf{R}^d)} \leqslant C \varepsilon^{\min(\ell,k)/2} \|\mathcal{K}\|_{W^{\ell,\infty}} \|u_1\|_{L^\infty([0,T];\Sigma^k)} \|u_2\|_{L^\infty([0,T];\Sigma^k)}.$$

In view of the computations performed in Section 2, this result has the following consequence.

Corollary 3.2. *Consider $\psi_{\rm app}^\varepsilon$ given by* (2.1)*, derived in Section 2, whose exact expression varies according to the cases $\alpha = 1$, $\alpha = 1/2$ or $\alpha = 0$. Let $T > 0$, and suppose $u_j \in C([0, T]; \Sigma^3)$. Then $\psi_{\rm app}^\varepsilon \in C([0, T]; \Sigma^3)$ satisfies $\psi_{{\rm app}|t=0}^\varepsilon = \psi_{|t=0}^\varepsilon$ and*

$$i\varepsilon \partial_t \psi_{\rm app}^\varepsilon + \frac{\varepsilon^2}{2} \Delta \psi_{\rm app}^\varepsilon = V\left(t, x\right) \psi_{\rm app}^\varepsilon + \sqrt{\varepsilon}\left(K * |\psi_{\rm app}^\varepsilon|^2\right) \psi_{\rm app}^\varepsilon + \varepsilon r^\varepsilon,$$

where $r^\varepsilon \in C(\mathbf{R}_+; L^2(\mathbf{R}^d))$ is such that there exists C independent of ε with

$$\sup_{t \in [0,T]} \|r^\varepsilon(t)\|_{L^2(\mathbf{R}^d)} \leqslant C\sqrt{\varepsilon}.$$

Remark 3.3. At this stage, the property $u_j \in C([0,T];\Sigma^3)$ is established in the cases $\alpha = 1$ and $\alpha = 1/2$. It will require some work to prove it in the case $\alpha = 0$; see Section 5. The assumptions of Corollary 3.2 are fulfilled, modulo the proof of Proposition 1.8.

Remark 3.4. Proposition 3.1 is a refinement of [12, Proposition 6.3], in the sense that the power of ε on the right hand side is as large as we wish, provided that $\mathcal{K}$ is sufficiently smooth, and that the functions u_1 and u_2 are sufficiently localized in space and frequency. Identifying precisely the norms of $\mathcal{K}$, u_1 and u_2, involved in order to get such an error estimate, will turn out to be crucial to prove Theorem 1.9, at the level of the bootstrap argument presented in Section 7.

3.1. **A microlocal property.** The proof of Proposition 3.1 is based on the following remark: the function that we integrate is localized away from the origin in *phase space*:

Lemma 3.5. *Suppose $(q_{10},p_{10}) \neq (q_{20},p_{20})$. In either of the cases $\alpha = 1$, $\alpha = 1/2$ or $\alpha = 0$, the following holds. For any $T > 0$, there exists $\eta > 0$ such that for all $t \in [0,T]$,*

$$|\delta q(t)| \geqslant \eta, \quad \text{or } |\delta p(t)| \geqslant \eta.$$

Proof. We argue by contradiction: if the result were not true, we could find a sequence $t_n \in [0,T]$ so that

$$|\delta q(t_n)| + |\delta p(t_n)| \underset{n\to\infty}{\longrightarrow} 0.$$

By compactness of $[0,T]$ and continuity of (q_j,p_j), there would exist $t_* \in [0,T]$ such that

$$q_1(t_*) = q_2(t_*), \quad p_1(t_*) = p_2(t_*).$$

In the cases $\alpha = 1$ and $\alpha = 1/2$, (q_j,p_j) is given by the classical Hamiltonian flow (1.3): uniqueness for (1.3) implies $(q_{10},p_{10}) = (q_{20},p_{20})$, hence a contradiction.

The case $\alpha = 0$ is a bit more delicate, since (q_j,p_j) is no longer given by a Hamiltonian flow. From (1.12), we infer:

$$\left\{\begin{aligned} &\frac{d(\delta q)}{dt} = \delta p,\\ &\frac{d(\delta p)}{dt} = \nabla V\left(t,q_2(t)\right) - \nabla V\left(t,q_1(t)\right) + \|a_1\|_{L^2}^2\left(\nabla K\left(-\delta q(t)\right) - \nabla K(0)\right)\\ &\qquad\qquad + \|a_2\|_{L^2}^2\left(\nabla K(0) - \nabla K\left(\delta q(t)\right)\right). \end{aligned}\right.$$

In view of Assumption 1.1, there exists C independent of t such that

$$\left|\frac{d(\delta q)}{dt}\right| + \left|\frac{d(\delta p)}{dt}\right| \leqslant C\left(|\delta p| + |\delta q|\right).$$

Gronwall's Lemma yields a contradiction, and the lemma is proved in the three cases. □

3.2. **Proof of Proposition 3.1.** From Lemma 3.5, if suffices to prove the estimate of Proposition 3.1 in either of the two cases $|\delta q(t)| \geqslant \eta$, or $|\delta p(t)| \geqslant \eta$.

First case. If $|\delta q(t)| \geqslant \eta$, we use Cauchy–Schwarz inequality to infer

$$\begin{aligned} |I^\varepsilon(t,y)| &\leqslant \|\mathcal{K}\|_{L^\infty} \int \frac{\langle z\rangle^k}{\langle z\rangle^k} |u_1(t,z)| \frac{\left\langle z + \frac{\delta q(t)}{\sqrt{\varepsilon}}\right\rangle^k}{\left\langle z + \frac{\delta q(t)}{\sqrt{\varepsilon}}\right\rangle^k} \left|u_2\left(t, z + \frac{\delta q(t)}{\sqrt{\varepsilon}}\right)\right| dz \\ &\leqslant \|\mathcal{K}\|_{L^\infty} \|u_1(t)\|_{\Sigma^k} \|u_2(t)\|_{\Sigma^k} \sup_{z\in\mathbf{R}^d} \langle z\rangle^{-k} \left\langle z + \frac{\delta q(t)}{\sqrt{\varepsilon}}\right\rangle^{-k}. \end{aligned}$$

In view of Peetre inequality (see e.g. [2, 41]),

$$\sup_{z\in\mathbf{R}^d}\langle z\rangle^{-k}\left\langle z+\frac{\delta q(t)}{\sqrt{\varepsilon}}\right\rangle^{-k}\leqslant C_k\left(\frac{\sqrt{\varepsilon}}{|\delta q(t)|}\right)^k\leqslant\frac{C_k}{\eta^k}\varepsilon^{k/2}.$$

Second case. If $|\delta p(t)|\geqslant\eta$, we perform repeated integrations by parts (like in the standard proof of the nonstationary phase lemma, see e.g. [2]) relying on the relation

$$e^{iz\cdot\delta p(t)/\sqrt{\varepsilon}}=-i\frac{\sqrt{\varepsilon}}{|\delta p(t)|^2}\sum_{\ell=1}^d(\delta p(t))_\ell\frac{\partial}{\partial z_\ell}\left(e^{iz\cdot\delta p(t)/\sqrt{\varepsilon}}\right).$$

Note that since we assume $\mathcal{K}\in W^{\ell,\infty}$ and $u_j\in\Sigma^k$, we perform no more than $\min(\ell,k)$ integrations by parts, and Cauchy–Schwarz inequality yields

$$|I^\varepsilon(t,y)|\leqslant\frac{1}{\eta^\ell}\|\mathcal{K}\|_{W^{\ell,\infty}}\|u_1(t)\|_{\Sigma^k}\|u_2(t)\|_{\Sigma^k}\varepsilon^{\min(\ell,k)/2}.$$

The proof of the proposition is complete.

4. Proof of convergence in the critical case

In this section, we complete the proof of Theorem 1.3. First, we recall that as a consequence of [17, 18], the system for the envelopes in the linear case is well-posed in Σ^k:

Lemma 4.1. *Let $k\in\mathbf{N}$, and $a\in\Sigma^k$. Then* (1.5) *has a unique solution $u\in C(\mathbf{R}_+;\Sigma^k)$. In addition, the following conservation holds:*

$$\|u(t)\|_{L^2(\mathbf{R}^d)}=\|a\|_{L^2(\mathbf{R}^d)},\quad\forall t\geqslant 0.$$

We infer that if $a_1,a_2\in\Sigma^3$, then u_1,u_2, given by (1.8), belong to $C(\mathbf{R}_+;\Sigma^3)$. Corollary 3.2 implies that $\psi^\varepsilon_{\rm app}$ satisfies

$$i\varepsilon\partial_t\psi^\varepsilon_{\rm app}+\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon_{\rm app}=V\psi^\varepsilon_{\rm app}+\varepsilon\left(K*|\psi^\varepsilon_{\rm app}|^2\right)\psi^\varepsilon_{\rm app}+\varepsilon r^\varepsilon;\quad\psi^\varepsilon_{\rm app}(0,x)=\psi^\varepsilon(0,x),$$

where the source term r^ε satisfies:

$$\forall T>0,\ \exists C>0,\quad\sup_{t\in[0,T]}\|r^\varepsilon(t)\|_{L^2(\mathbf{R}^d)}\leqslant C\sqrt{\varepsilon}.$$

Denote by $w^\varepsilon=\psi^\varepsilon-\psi^\varepsilon_{\rm app}$ the error term. It satisfies

$$i\varepsilon\partial_t w^\varepsilon+\frac{\varepsilon^2}{2}\Delta w^\varepsilon=Vw^\varepsilon+\varepsilon\left(\left(K*|\psi^\varepsilon|^2\right)\psi^\varepsilon-\left(K*|\psi^\varepsilon_{\rm app}|^2\right)\psi^\varepsilon_{\rm app}\right)-\varepsilon r^\varepsilon,$$

with $w^\varepsilon_{|t=0}=0$. Writing

$$\begin{aligned}\left(K*|\psi^\varepsilon|^2\right)\psi^\varepsilon-&\left(K*|\psi^\varepsilon_{\rm app}|^2\right)\psi^\varepsilon_{\rm app}\\&=\left(K*|w^\varepsilon+\psi^\varepsilon_{\rm app}|^2\right)\left(w^\varepsilon+\psi^\varepsilon_{\rm app}\right)-\left(K*|\psi^\varepsilon_{\rm app}|^2\right)\psi^\varepsilon_{\rm app}\\&=\left(K*|w^\varepsilon+\psi^\varepsilon_{\rm app}|^2\right)w^\varepsilon+\left(K*\left(|w^\varepsilon+\psi^\varepsilon_{\rm app}|^2-|\psi^\varepsilon_{\rm app}|^2\right)\right)\psi^\varepsilon_{\rm app},\end{aligned}$$

energy estimates yield, for $t\in[0,T]$, and since ψ^ε, $\psi^\varepsilon_{\rm app}$ (hence w^ε) are uniformly bounded in $L^\infty(\mathbf{R}_+;L^2(\mathbf{R}^d))$:

$$\begin{aligned}
\|w^\varepsilon(t)\|_{L^2} &\leqslant \int_0^t \left\|K*\left(|w^\varepsilon+\psi^\varepsilon_{\rm app}|^2-|\psi^\varepsilon_{\rm app}|^2\right)(s)\right\|_{L^\infty}\|\psi^\varepsilon_{\rm app}(s)\|_{L^2}ds\\
&\quad+\int_0^t\|r^\varepsilon(s)\|_{L^2}ds\\
&\leqslant C\int_0^t\left\|\left(|w^\varepsilon+\psi^\varepsilon_{\rm app}|^2-|\psi^\varepsilon_{\rm app}|^2\right)(s)\right\|_{L^1}ds+\int_0^t\|r^\varepsilon(s)\|_{L^2}ds\\
&\leqslant C\int_0^t\|w^\varepsilon(s)\|_{L^2}+\int_0^t\|r^\varepsilon(s)\|_{L^2}ds,
\end{aligned}$$

for $C>0$ independent of $\varepsilon\in(0,1]$ and $t\geqslant 0$. Theorem 1.3 is then a consequence of Gronwall's Lemma.

Remark 4.2. Assuming that we have proved the property $u_j\in C([0,T];\Sigma^3)$ in the case $\alpha=0$, which will stem from Proposition 1.8, the conclusion of Corollary 3.2 holds. However, the estimate given by the above approach is not satisfactory in the cases $\alpha=1/2$ and $\alpha=0$. We could prove this way:

$$\|\psi^\varepsilon(t)-\psi^\varepsilon_{\rm app}(t)\|_{L^2}\leqslant C\sqrt{\varepsilon}e^{Ct/\varepsilon^{1-\alpha}},\quad t\in[0,T],$$

for $\alpha=1/2$ and $\alpha=0$, respectively. Contrary to the case $\alpha=1$ (where Gronwall's Lemma yields a similar estimate), we can only conclude that $\psi^\varepsilon-\psi^\varepsilon_{\rm app}$ is goes to zero on a small time interval: there exist $c>0$ and $\theta>0$ such that

$$\sup_{0\leqslant t\leqslant c\varepsilon^{1-\alpha}|\ln\varepsilon|^\theta}\|\psi^\varepsilon(t)-\psi^\varepsilon_{\rm app}(t)\|_{L^2}\underset{\varepsilon\to 0}{\longrightarrow}0.$$

Corollary 3.2 is a consistency result, which is not enough to infer convergence. This can be understood as a feature of supercritical regimes: a different approach is needed, which requires more regularity from V, K, and the initial data a_j.

5. THE ENVELOPE EQUATIONS IN THE CASE $\alpha=0$

In this section, we prove Proposition 1.8. We first remark that the last two terms in each equation involved in (1.13) correspond to purely time-dependent potentials, and can be treated thanks to the gauge transforms

$$\left\{\begin{aligned}
v_1(t,y)&=u_1(t,y)\exp\Big(-i\int_0^t\int\left\langle z,\nabla^2K(0)z\right\rangle|u_1(s,z)|^2dzds\\
&\qquad\qquad -i\int_0^t\int\left\langle z,\nabla^2K\left(\delta q(s)\right)z\right\rangle|u_2(s,z)|^2dzds\Big),\\
v_2(t,y)&=u_2(t,y)\exp\Big(-i\int_0^t\int\left\langle z,\nabla^2K(0)z\right\rangle|u_2(s,z)|^2dzds\\
&\qquad\qquad -i\int_0^t\int\left\langle z,\nabla^2K\left(-\delta q(s)\right)z\right\rangle|u_1(s,z)|^2dzds\Big).
\end{aligned}\right.\tag{5.1}$$

Since K is real-valued, we have $|v_j(t,y)| = |u_j(t,y)|$, and (5.1) is equivalent to

$$\text{(5.2)}\quad \begin{cases} u_1(t,y) = v_1(t,y)\exp\Big(i\int_0^t\int \left\langle z, \nabla^2 K(0) z\right\rangle |v_1(s,z)|^2 dz ds \\ \qquad\qquad\qquad + i\int_0^t\int \left\langle z, \nabla^2 K\left(\delta q(s)\right) z\right\rangle |v_2(s,z)|^2 dz ds\Big), \\ u_2(t,y) = v_2(t,y)\exp\Big(i\int_0^t\int \left\langle z, \nabla^2 K(0) z\right\rangle |v_2(s,z)|^2 dz ds \\ \qquad\qquad\qquad + i\int_0^t\int \left\langle z, \nabla^2 K\left(-\delta q(s)\right) z\right\rangle |v_1(s,z)|^2 dz ds\Big). \end{cases}$$

Formally, (u_1,u_2) solves (1.13) if and only if (v_1,v_2) solves

$$\text{(5.3)}\quad \begin{cases} i\partial_t v_1 + \frac{1}{2}\Delta v_1 = \frac{1}{2}\left\langle y, M_1(t)y\right\rangle v_1 - \left\langle \nabla^2 K(0) G_1(t), y\right\rangle v_1 \\ \qquad\qquad\qquad - \left\langle \nabla^2 K\left(\delta q(t)\right) G_2(t), y\right\rangle v_1, \\ i\partial_t v_2 + \frac{1}{2}\Delta v_2 = \frac{1}{2}\left\langle y, M_2(t)y\right\rangle v_2 - \left\langle \nabla^2 K(0) G_2(t), y\right\rangle v_2 \\ \qquad\qquad\qquad - \left\langle \nabla^2 K\left(-\delta q(t)\right) G_1(t), y\right\rangle v_2, \end{cases}$$

with the same initial data, $v_{j|t=0} = a_j$, $j = 1,2$, where the bounded, symmetric matrices M_1 and M_2 are defined in (1.15) and (1.16), respectively, and where we have kept the notation

$$G_j(t) = \int z|v_j(t,z)|^2 dz.$$

Note that the terms involved in the gauge transforms are well defined when the functions are in Σ^k with $k \geqslant 1$, so Proposition 1.8 stems from the following:

Proposition 5.1. *Let (q_1,p_1,q_2,p_2) be given by Lemma 1.6, and $a_1,a_2 \in \Sigma^k$ with $k \geqslant 1$. Then* (5.3) *has a unique solution $(v_1,v_2) \in C(\mathbf{R}_+;\Sigma^k)$ with initial data (a_1,a_2). In addition, the following conservations hold:*

$$\|v_j(t)\|_{L^2(\mathbf{R}^d)} = \|a_j\|_{L^2(\mathbf{R}^d)}, \quad \forall t \geqslant 0,\ j = 1,2.$$

Proof. The main difficulty is that since the last two terms in each equation involve time dependent potentials which are unbounded in y, they cannot be treated by perturbative arguments. So to construct a local solution, we modify the standard Picard iterative scheme in the same fashion as in [9], to consider

$$\text{(5.4)}\quad \begin{cases} i\partial_t v_1^{(n)} + \frac{1}{2}\Delta v_1^{(n)} = \frac{1}{2}\left\langle y, M_1(t)y\right\rangle v_1^{(n)} - \left\langle \nabla^2 K(0) G_1^{(n-1)}(t), y\right\rangle v_1^{(n)} \\ \qquad\qquad\qquad - \left\langle \nabla^2 K\left(\delta q(t)\right) G_2^{(n-1)}(t), y\right\rangle v_1^{(n)}, \\ i\partial_t v_2^{(n)} + \frac{1}{2}\Delta v_2^{(n)} = \frac{1}{2}\left\langle y, M_2(t)y\right\rangle v_2^{(n)} - \left\langle \nabla^2 K(0) G_2^{(n-1)}(t), y\right\rangle v_2^{(n)} \\ \qquad\qquad\qquad - \left\langle \nabla^2 K\left(-\delta q(t)\right) G_1^{(n-1)}(t), y\right\rangle v_2^{(n)}, \end{cases}$$

with $v^{(n)}_{j|t=0} = a_j$ for all n, $v_j^{(0)}(t,y) = a_j(y)$, and

$$G_j^{(k)}(t) = \int_{\mathbf{R}^d} z\left|v_j^{(k)}(s,z)\right|^2 ds.$$

At each step, we solve a decoupled system of linear equation, with time dependent potentials which are at most quadratic in space. If $G_1^{(n-1)}, G_2^{(n-1)} \in L^\infty_{\rm loc}(\mathbf{R}_+)$, [18] ensures the existence of $v_1^{(n)}, v_2^{(n)} \in C(\mathbf{R}_+; L^2(\mathbf{R}^d))$. In addition, we have

$$\left\| v_j^{(n)}(t) \right\|_{L^2(\mathbf{R}^d)} = \|a_j\|_{L^2(\mathbf{R}^d)} \quad \forall t \geqslant 0,\ j=1,2.$$

Applying the operators y and ∇ to (5.4) yields a closed system of estimates, from which we infer that $v_j^{(n)} \in C(\mathbf{R}_+;\Sigma)$, hence $G_j^{(n)} \in L^\infty_{\rm loc}(\mathbf{R}_+)$. Therefore, the scheme is well-defined. Higher order regularity can be proven similarly: for $k \geqslant 1$, by applying k times the operators y and ∇ to (5.4), we check that $v_1^{(n)}, v_2^{(n)} \in C(\mathbf{R}_+;\Sigma^k)$. As a matter of fact, due to the particular structure of (5.4), the only informations needed to prove this property are $a_j \in \Sigma^k$ and $v_j^{(n-1)} \in C(\mathbf{R}_+;\Sigma)$.

To prove the convergence of this scheme we need more precise (uniform in n) estimates. A general computation shows that if v solves

$$i\partial_t v + \frac{1}{2}\Delta v = \frac{1}{2}\left\langle y, M(t)y\right\rangle v + F(t)\cdot y\, v,$$

where $M(t)$ is a real-valued, symmetric matrix, and $F(t)$ is a real-valued vector, then $G(t) = \displaystyle\int z|v(t,z)|^2dz$ satisfies formally

$$\begin{aligned}
\dot G(t) &= \operatorname{Im}\int \bar v \nabla v =: J(t),\\
\dot J(t) &= -\int \left(M(t)y + F(t)\right)|v(t,y)|^2 dy = -M(t)G(t) - F(t)\|v\|_{L^2}^2,
\end{aligned}$$

where the last expression uses implicitly the fact that the L^2-norm of v is independent of time. We have in particular:

$$\ddot G(t) + M(t)G(t) = -\|v\|^2_{L^2}F(t).$$

In our case, this yields:

$$\ddot G_1^{(n)} + M_1(t)G_1^{(n)} = \|a_1\|^2_{L^2}\nabla^2K(0)G_1^{(n-1)} + \|a_2\|^2_{L^2}\nabla^2 K\left(\delta q(t)\right)G_2^{(n-1)}, \tag{5.5}$$

$$\ddot G_2^{(n)} + M_2(t)G_2^{(n)} = \|a_2\|^2_{L^2}\nabla^2K(0)G_2^{(n-1)} + \|a_1\|^2_{L^2}\nabla^2 K\left(-\delta q(t)\right)G_1^{(n-1)}. \tag{5.6}$$

Let

$$f_n(t) = \left|\dot G_1^{(n)}(t)\right|^2 + \left|\dot G_2^{(n)}(t)\right|^2 + \left|G_1^{(n)}(t)\right|^2 + \left|G_2^{(n)}(t)\right|^2.$$

We have

$$\begin{aligned}
\dot f_n(t) &\leqslant 2\sum_{j=1,2}\left(\left|\dot G_j^{(n)}(t)\right|\left|\ddot G_j^{(n)}(t)\right| + \left|\dot G_j^{(n)}(t)\right|\left|G_j^{(n)}(t)\right|\right)\\
&\leqslant C f_n(t) + C\sum_{j=1,2}\left|G_j^{(n-1)}(t)\right|^2,
\end{aligned}$$

for some C independent of t and n, since $\nabla^2 V, \nabla^2 K \in L^\infty$, and where we have used (5.5)-(5.6) and Young's inequality. By Gronwall's Lemma, we infer

$$f_n(t) \leqslant f_n(0)e^{Ct} + C\int_0^t e^{C(t-s)}f_{n-1}(s)ds.$$

With our definition of the scheme, $f_n(0)$ does not depend on n:

$$f_n(0) = \sum_{j=1,2} \left(\left| \mathrm{Im} \int \bar{a}_j \nabla a_j \right|^2 + \left| \int z |a_j(z)|^2 dz \right|^2 \right) =: C_0.$$

Therefore,

$$f_n(t) \leqslant C_0 e^{Ct} + C \int_0^t e^{C(t-s)} f_{n-1}(s) ds,$$

and by induction, we infer

$$f_n(t) \leqslant 2C_0 e^{3Ct}, \quad t \geqslant 0.$$

By using energy estimates (applying the operators y and ∇ successively to the equations), we infer that there exists C_1 independent of $t \geqslant 0$ and n such that

$$\sum_{j=1,2} \left\| v_j^{(n)}(t) \right\|_{\Sigma^k} \leqslant C_1 e^{C_1 t}.$$

The convergence of the sequence $(v_1^{(n)}, v_2^{(n)})$ then follows: we check that v_n converges in $C([0,T];\Sigma)$ if $T > 0$ is sufficiently small. To simplify the presentation, we present this argument in the case of a single envelope equation, the case of (5.4) bearing no extra difficulty:

$$i\partial_t v^{(n)} + \frac{1}{2}\Delta v^{(n)} = \frac{1}{2} \langle y, M(t) y \rangle v^{(n)} + \left\langle Q(t) G^{(n-1)}(t), y \right\rangle v^{(n)}, \tag{5.7}$$

where $Q(t)$ is a real-valued, symmetric matrix, with $Q \in L^\infty(\mathbf{R}_+)$. Denoting by

$$H(t) = -\frac{1}{2}\Delta + \frac{1}{2} \langle y, M(t) y \rangle,$$

we have

$$\begin{aligned} i\partial_t \left(v^{(n)} - v^{(n-1)} \right) &= H \left(v^{(n)} - v^{(n-1)} \right) + \left\langle Q(t) G^{(n-1)}(t), y \right\rangle \left(v^{(n)} - v^{(n-1)} \right) \\ &\quad + \left\langle Q(t) \left(G^{(n-1)}(t) - G^{(n-2)}(t) \right), y \right\rangle v^{(n-1)} \end{aligned}$$

Energy estimates and the above uniform bound yield

$$\begin{aligned} \left\| v^{(n)}(t) - v^{(n-1)}(t) \right\|_{L^2} &\leqslant C \int_0^t \left| G^{(n-1)}(s) - G^{(n-2)}(s) \right| ds \\ &\leqslant C \int_0^t e^{C_1 s} \left\| v^{(n-1)}(s) - v^{(n-2)}(s) \right\|_\Sigma ds \end{aligned}$$

By applying the operators y and ∇ to (5.7), we obtain similarly:

$$\left\| v^{(n)}(t) - v^{(n-1)}(t) \right\|_\Sigma \leqslant C \int_0^t e^{C_1 s} \left\| v^{(n-1)}(s) - v^{(n-2)}(s) \right\|_\Sigma ds.$$

Therefore, we can find $T > 0$ such that the sequence $v^{(n)}$ converges in $C([0,T];\Sigma)$, to $v \in C([0,T];\Sigma^k)$. The uniform bounds for the sequence $v^{(n)}$ imply that v is global in time: $v \in C(\mathbf{R}_+;\Sigma^k)$, with Σ^k-norms growing at most exponentially in time. □

6. CONVERGENCE IN SUPERCRITICAL CASES: SCHEME OF THE PROOF

We present the proof of Theorem 1.9 in details; the proof of Theorem 1.5 can easily be adapted (see Remark 6.2 below).

6.1. **The general picture.** In [3, 9], where the case of only one wave packet is considered, the proof of stability relies on a change of unknown function: writing

$$\psi^\varepsilon(t,x) = \varepsilon^{-d/4} u^\varepsilon\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}\right) e^{i(S^\varepsilon(t)+(x-q(t))\cdot p(t))/\varepsilon},$$

with S^ε, q and p as given by the construction of the approximate solution, it is *equivalent* to work on ψ^ε or u^ε in order to prove an error estimate, since

$$\|\psi^\varepsilon(t) - \psi^\varepsilon_{\rm app}(t)\|_{L^2(\mathbf{R}^d)} = \|u^\varepsilon(t) - u(t)\|_{L^2(\mathbf{R}^d)}.$$

Passing from the unknown ψ^ε to u^ε amounts to using very fine geometric properties related to the dynamics: the modified action S^ε, and (q,p). One changes the origin in phase space, to work in the moving frame associated to the wave packet. In the case of two wave packets, there are two moving frames, so the approach that we follow is different. We construct a solution to (1.1) of the form

$$\psi^\varepsilon(t,x) = \varepsilon^{-d/4} \sum_{j=1,2} u_j^\varepsilon\left(t, \frac{x-q_j(t)}{\sqrt{\varepsilon}}\right) e^{i\left(S_j^\varepsilon(t)+p_j(t)\cdot(x-q_j(t))\right)/\varepsilon}, \tag{6.1}$$

where the quantities (q_j,p_j) and S_j^ε are those given by the construction of $\psi^\varepsilon_{\rm app}$, so we consider two unknown functions, u_1^ε and u_2^ε. To do so, we derive formally a system for $(u_1^\varepsilon, u_2^\varepsilon)$, which is morally equivalent to (1.1): rigorously, the solution to this system yields a solution to (1.1), and by uniqueness for (1.1), the relation (6.1) is valid. In turn, the construction of the solution $(u_1^\varepsilon, u_2^\varepsilon)$ on arbitrary time intervals relies on a bootstrap argument, consisting of a comparison of a modification of $(u_1^\varepsilon, u_2^\varepsilon)$ with (u_1,u_2), defined in (1.13). This modification eventually corresponds to the presence of the phase shifts θ_j in Theorem 1.9.

In order to shorten the formulas, we consider indices in $\mathbf{Z}/2\mathbf{Z}$: typically, q_j stands for q_1 whenever $j=1$ or 3. Plugging (6.1) into (1.1) in the case $\alpha=0$, we find:

$$i\varepsilon\partial_t\psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon - V\psi^\varepsilon - \left(K*|\psi^\varepsilon|^2\right)\psi^\varepsilon = \varepsilon^{-d/4}\sum_{j=1,2} e^{i\phi_j^\varepsilon(t,x)} N_j^\varepsilon,$$

where we have denoted

$$\begin{aligned}
&\phi_j^\varepsilon(t,x) = S_j^\varepsilon(t) + p_j(t)\cdot(x-q_j(t)),\\
&N_j^\varepsilon = i\varepsilon\partial_t u_j^\varepsilon - u_j^\varepsilon\partial_t\phi_j^\varepsilon + \frac{\varepsilon}{2}\Delta u_j^\varepsilon - \frac{|p_j(t)|^2}{2}u_j^\varepsilon - V\left(t, q_j(t)+y_j\sqrt{\varepsilon}\right)u_j^\varepsilon - \tilde V_j^{\rm NL} u_j^\varepsilon,\\
&\tilde V_j^{\rm NL}(t,y_j) = \int K\left(\sqrt{\varepsilon}(y_j-z)\right)|u_j^\varepsilon(t,z)|^2dz\\
&\qquad\qquad + \int K\left(q_j-q_{j+1}+\sqrt{\varepsilon}(y_j-z)\right)|u_{j+1}^\varepsilon(t,z)|^2dz\\
&\qquad\qquad + 2\,\mathrm{Re}\, e^{i\left(S_j^\varepsilon - S_{j+1}^\varepsilon - q_j\cdot p_j + q_{j+1}\cdot p_{j+1}\right)/\varepsilon}\times\\
&\qquad \times\int K\left(\sqrt{\varepsilon}(y_j-z)\right)e^{iz\cdot(p_j-p_{j+1})/\sqrt{\varepsilon}}u_j^\varepsilon(t,z)\overline{u}_{j+1}^\varepsilon\left(t, z+\frac{q_j-q_{j+1}}{\sqrt{\varepsilon}}\right)dz.
\end{aligned}$$

Note that the computations which we do not detail correspond to the computations presented in Section 2, up to the fact that now, we do not perform Taylor expansions for V or K. As in Section 2, we distinguish the variables y_1 and y_2.

Our approach consists in considering the set of coupled, nonlinear equations

$$N_1^\varepsilon = N_2^\varepsilon = 0.$$

It is important to notice at this stage of the construction that this system conserves formally the L^2 norms: since we naturally impose $u^\varepsilon_{j|t=0} = a_j$, we have

$$\|u_j^\varepsilon(t)\|_{L^2(\mathbf{R}^d)} = \|a_j\|_{L^2(\mathbf{R}^d)}, \quad j = 1, 2,$$

as long as $(u_1^\varepsilon, u_2^\varepsilon)$ is well defined. This property is the reason why we can perform important reductions in the system. Taking into account the expression of the modified actions S_j^ε, we find:

$$\begin{aligned}
N_j^\varepsilon &= i\varepsilon\partial_t u_j^\varepsilon - u_j^\varepsilon \left(\dot{S}_j^\varepsilon(t) + \sqrt{\varepsilon}\dot{p}_j(t)\cdot y_j - p_j(t)\cdot \dot{q}_j(t)\right) \\
&\quad + \frac{\varepsilon}{2}\Delta u_j^\varepsilon - \frac{|p_j(t)|^2}{2}u_j^\varepsilon - V\left(t, q_j(t) + y_j\sqrt{\varepsilon}\right)u_j^\varepsilon - \tilde{V}_j^{\mathrm{NL}}(t,y_j)u_j^\varepsilon \\
&= i\varepsilon\partial_t u_j^\varepsilon - \left(\sqrt{\varepsilon}\dot{p}_j(t)\cdot y_j - p_j(t)\cdot\dot{q}_j(t)\right)u_j^\varepsilon \\
&\quad - \left(\frac{1}{2}|p_j|^2 - V(t,q_j) - K(0)\|a_j\|_{L^2} - K(q_j - q_{j+1})\|a_{j+1}\|^2_{L^2}\right)u_j^\varepsilon \\
&\quad + \left(\sqrt{\varepsilon}\nabla K(0)\cdot G_j(t) + \sqrt{\varepsilon}\nabla K(q_j - q_{j+1})\cdot G_{j+1}(t)\right)u_j^\varepsilon \\
&\quad + \frac{\varepsilon}{2}\Delta u_j^\varepsilon - \frac{|p_j(t)|^2}{2}u_j^\varepsilon - V\left(t, q_j(t) + y_j\sqrt{\varepsilon}\right)u_j^\varepsilon - \tilde{V}_j^{\mathrm{NL}}(t,y_j)u_j^\varepsilon \\
&= i\varepsilon\partial_t u_j^\varepsilon + \frac{\varepsilon}{2}\Delta u_j^\varepsilon - \sqrt{\varepsilon}\dot{p}_j(t)\cdot y_j u_j^\varepsilon \\
&\quad - \left(V\left(t, q_j(t) + y_j\sqrt{\varepsilon}\right) - V(t,q_j)\right)u_j^\varepsilon \\
&\quad - \left(\tilde{V}_j^{\mathrm{NL}}(t,y_j) - K(0)\|a_j\|_{L^2} - K(q_j - q_{j+1})\|a_{j+1}\|^2_{L^2}\right)u_j^\varepsilon \\
&\quad + \left(\sqrt{\varepsilon}\nabla K(0)\cdot G_j(t) + \sqrt{\varepsilon}\nabla K(q_j - q_{j+1})\cdot G_{j+1}(t)\right)u_j^\varepsilon.
\end{aligned}$$

If we now take into account the expression of $\dot{p}_j$, given in (1.12), we infer:

$$\begin{aligned}
N_j^\varepsilon &= i\varepsilon\partial_t u_j^\varepsilon + \frac{\varepsilon}{2}\Delta u_j^\varepsilon \\
&\quad + \sqrt{\varepsilon}y_j\cdot\left(\nabla V(t,q_j) + \|a_j\|^2_{L^2}\nabla K(0) + \|a_{j+1}\|^2_{L^2}\nabla K(q_j - q_{j+1})\right)u_j^\varepsilon \\
&\quad - \left(V\left(t, q_j(t) + y_j\sqrt{\varepsilon}\right) - V(t,q_j)\right)u_j^\varepsilon \\
&\quad - \left(\tilde{V}_j^{\mathrm{NL}}(t,y_j) - K(0)\|a_j\|^2_{L^2} - K(q_j - q_{j+1})\|a_{j+1}\|^2_{L^2}\right)u_j^\varepsilon \\
&\quad + \left(\sqrt{\varepsilon}\nabla K(0)\cdot G_j(t) + \sqrt{\varepsilon}\nabla K(q_j - q_{j+1})\cdot G_{j+1}(t)\right)u_j^\varepsilon.
\end{aligned}$$

It is now natural to introduce the following notations:

$$\begin{aligned}
V_j^\varepsilon(t,y_j) &= \frac{1}{\varepsilon}\left(V\left(t, q_j(t) + y_j\sqrt{\varepsilon}\right) - V\left(t,q_j(t)\right) - \sqrt{\varepsilon}y_j\cdot\nabla V\left(t,q_j(t)\right)\right), \\
K_{j,\mathrm{diag}}^\varepsilon(t,y_j) &= \frac{1}{\varepsilon}\left(K\left(\sqrt{\varepsilon}y_j\right) - K(0) - \sqrt{\varepsilon}y_j\cdot\nabla K(0)\right), \\
K_{j,\mathrm{off}}^\varepsilon(t,y_j) &= \frac{1}{\varepsilon}\left(K\left(q_j - q_{j+1} + \sqrt{\varepsilon}y_j\right) - K(q_j - q_{j+1}) - \sqrt{\varepsilon}y_j\cdot\nabla K(q_j - q_{j+1})\right).
\end{aligned}$$

From the assumptions on V and K, there exists $C > 0$ independent of $\varepsilon \in (0,1]$ such that

$$\sum_{2\leqslant|\alpha|\leqslant 6}\left\|\partial_{y_j}^\alpha V_j^\varepsilon(t)\right\|_{L^\infty} + \sum_{2\leqslant|\alpha|\leqslant 6}\left\|\partial_{y_j}^\alpha K_j^\varepsilon(t)\right\|_{L^\infty} \leqslant C, \tag{6.2}$$

where K_j^ε stands for $K^\varepsilon_{j,\rm diag}$ or $K^\varepsilon_{j,\rm off}$, indistinctly. In view of Taylor's formula, we have:

$$V_j^\varepsilon(t,y_j) = \int_0^1 \left\langle y_j, \nabla^2 V\left(t, q_j(t)+\theta y_j\sqrt{\varepsilon}\right) y_j\right\rangle (1-\theta)d\theta, \tag{6.3}$$

$$K^\varepsilon_{j,\rm diag}(t,y_j) = \int_0^1 \left\langle y_j, \nabla^2 K\left(\theta y_j\sqrt{\varepsilon}\right) y_j\right\rangle (1-\theta)d\theta, \tag{6.4}$$

$$K^\varepsilon_{j,\rm off}(t,y_j) = \int_0^1 \left\langle y_j, \nabla^2 K\left(q_j(t)-q_{j+1}(t)+\theta y_j\sqrt{\varepsilon}\right) y_j\right\rangle (1-\theta)d\theta. \tag{6.5}$$

Therefore, we consider the coupled system (coupling is present through K_j^ε):

$$\left\{\begin{aligned} i\partial_t u_j^\varepsilon + \frac{1}{2}\Delta u_j^\varepsilon &= V_j^\varepsilon(t,y_j)u_j^\varepsilon + \left(K^\varepsilon_{j,\rm diag} * |u_j^\varepsilon|^2\right) u_j^\varepsilon + \left(K^\varepsilon_{j,\rm off} * |u_{j+1}^\varepsilon|^2\right) u_j^\varepsilon \\ &\quad -\frac{1}{\sqrt{\varepsilon}}\nabla K(0)\cdot\left(\int z\left(|u_j^\varepsilon(t,z)|^2 - |u_j(t,z)|^2\right)dz\right)u_j^\varepsilon \\ &\quad -\frac{1}{\sqrt{\varepsilon}}\nabla K(q_j-q_{j+1})\cdot\left(\int z\left(|u_{j+1}^\varepsilon(t,z)|^2 - |u_{j+1}(t,z)|^2\right)dz\right)u_j^\varepsilon \\ &\quad +\frac{1}{\varepsilon}\left(2\,\mathrm{Re}\, W_j^\varepsilon(t,y_j)\right)u_j^\varepsilon, \end{aligned}\right. \tag{6.6}$$

with

$$\begin{aligned} W_j^\varepsilon(t,y_j) &= e^{i\left(S_j^\varepsilon - S_{j+1}^\varepsilon - q_j\cdot p_j + q_{j+1}\cdot p_{j+1}\right)/\varepsilon}\times \\ &\times \int K\left(\sqrt{\varepsilon}(y_j-z)\right)e^{iz\cdot(p_j-p_{j+1})/\sqrt{\varepsilon}}u_j^\varepsilon(t,z)\overline{u}_{j+1}^\varepsilon\left(t, z+\frac{q_j-q_{j+1}}{\sqrt{\varepsilon}}\right)dz. \end{aligned}$$

6.2. **Further simplification and bootstrap argument.** The last three terms in (6.6) are singular in the limit $\varepsilon\to 0$. However, the singularity of the last term is expected to be artificial, since in view of Proposition 3.1, it should even be small, provided we have uniform estimates for u_j^ε in Σ^3. The other two singular terms have an interesting feature: they are real-valued, and depend only on time, so we can treat them thanks to a gauge transform. Introduce

$$\begin{aligned} i\partial_t \tilde u_j^\varepsilon + \frac{1}{2}\Delta \tilde u_j^\varepsilon &= V_j^\varepsilon(t,y_j)\tilde u_j^\varepsilon + \left(K^\varepsilon_{j,\rm diag} * |\tilde u_j^\varepsilon|^2\right) \tilde u_j^\varepsilon + \left(K^\varepsilon_{j,\rm off} * |\tilde u_{j+1}^\varepsilon|^2\right) \tilde u_j^\varepsilon \\ &\quad + \frac{1}{\varepsilon}\left(2\,\mathrm{Re}\,\tilde W_j^\varepsilon\right)\tilde u_j^\varepsilon, \end{aligned} \tag{6.7}$$

with initial data $\tilde u^\varepsilon_{j|t=0} = a_j$, and where we have denoted

$$\begin{aligned} \tilde W_j^\varepsilon &= e^{i\left(S_j^\varepsilon - S_{j+1}^\varepsilon - q_j\cdot p_j + q_{j+1}\cdot p_{j+1}\right)/\varepsilon} e^{i(\theta_j^\varepsilon-\theta_{j+1}^\varepsilon)}\times \\ &\times \int K\left(\sqrt{\varepsilon}(y_j-z)\right)e^{iz\cdot(p_j-p_{j+1})/\sqrt{\varepsilon}}\tilde u_j^\varepsilon(t,z)\overline{\tilde u}_{j+1}^\varepsilon\left(t, z+\frac{q_j-q_{j+1}}{\sqrt{\varepsilon}}\right)dz, \end{aligned}$$

with

$$\begin{aligned} \theta_j^\varepsilon(t) &= \frac{1}{\sqrt{\varepsilon}}\int_0^t \nabla K(0)\cdot\left(\int z\left(|\tilde u_j^\varepsilon(s,z)|^2 - |u_j(s,z)|^2\right)dz\right)ds \\ &\quad + \frac{1}{\sqrt{\varepsilon}}\int_0^t \nabla K(q_j(s)-q_{j+1}(s))\cdot\left(\int z\left(|\tilde u_{j+1}^\varepsilon(s,z)|^2 - |u_{j+1}(s,z)|^2\right)dz\right)ds. \end{aligned}$$

We then have: $u_j^\varepsilon(t,y) = \tilde u_j^\varepsilon(t,y)e^{i\theta_j^\varepsilon(t)}$. Note that $|u_j^\varepsilon| = |\tilde u_j^\varepsilon|$, so it is equivalent to pass from u_j^ε to $\tilde u_j^\varepsilon$, or from $\tilde u_j^\varepsilon$ to u_j^ε. In view of these reductions, *in a first approximation*, Theorem 1.9 stems from:

Theorem 6.1. *Let $d \geqslant 1$ and $a_1, a_2 \in \Sigma^6$. Assume that V and K are real-valued and:*

$$V \in C^6(\mathbf{R}_+ \times \mathbf{R}^d; \mathbf{R}), \quad \textit{and} \quad \partial_x^\beta V \in L^\infty\left(\mathbf{R}_+ \times \mathbf{R}^d\right), \quad 2 \leqslant |\beta| \leqslant 6.$$
$$K \in W^{6,\infty}(\mathbf{R}^d; \mathbf{R}).$$

Let $T > 0$. There exists $\varepsilon_0 > 0$ such that for $\varepsilon \in (0, \varepsilon_0]$, (6.7) *has a unique solution $(\tilde{u}_1^\varepsilon, \tilde{u}_2^\varepsilon) \in C([0,T]; \Sigma^3)^2$. Moreover, there exists C independent of $\varepsilon \in (0, \varepsilon_0]$ such that*

$$\sup_{t\in[0,T]} \|\tilde{u}_1^\varepsilon(t) - u_1(t)\|_{\Sigma^3} + \sup_{t\in[0,T]} \|\tilde{u}_2^\varepsilon(t) - u_2(t)\|_{\Sigma^3} \leqslant C\sqrt{\varepsilon}. \tag{6.8}$$

Several comments are in order. First, this result implies that for $j = 1, 2$, $\dot{\theta}_j^\varepsilon$ is bounded on $[0, T]$, uniformly in ε. To get the result stated in Theorem 1.9, we will prove that the functions θ_j^ε converge as $\varepsilon \to 0$, by performing a second order asymptotic expansion of $(\tilde{u}_1^\varepsilon, \tilde{u}_2^\varepsilon)$ (Theorem 6.1 yields the first order asymptotic expansion).

Even in the case of a single wave packet, this result is new, since we do not assume $\nabla K(0) = 0$. In that case, the last term in (6.7) vanishes, and the proof that we present below becomes simpler.

The proof is based on a bootstrap argument detailed in Section 7. For fixed $\varepsilon > 0$, (6.7) has a unique, local solution: $(\tilde{u}_1^\varepsilon, \tilde{u}_2^\varepsilon) \in C([0, \tau^\varepsilon]; \Sigma^3)^2$, for some $\tau^\varepsilon > 0$. This can be proven by adapting the approach presented in Section 5. To prove the theorem, we use energy estimates to prove that so long as $(\tilde{u}_1^\varepsilon, \tilde{u}_2^\varepsilon)$ is bounded in $C([0,\tau]; \Sigma^3)^2$, $\tau^\varepsilon \leqslant \tau \leqslant T$, (6.8) is true. Therefore, choosing $\varepsilon_0 > 0$ sufficiently small, $(\tilde{u}_1^\varepsilon, \tilde{u}_2^\varepsilon) \in C([0,T]; \Sigma^3)^2$ for $\varepsilon \in (0, \varepsilon_0]$, and (6.8) is satisfied.

The reason why we work in Σ^3 and not in a larger space is that we want to be able to neglect $\tilde{W}_j^\varepsilon$: because of the singular factor $1/\varepsilon$ in front of the last term in (6.7), we need to prove $\tilde{W}_j^\varepsilon = o(\varepsilon)$, and Proposition 3.1 suggests that we need to work in Σ^3, in which case $\tilde{W}_j^\varepsilon = \mathcal{O}(\varepsilon^{3/2})$. To differentiate V_j^ε and K_j^ε three times (we work in Σ^3), (6.3)–(6.5) and Proposition 3.1 suggest to work with the regularity stated in Theorem 6.1 (the same as in Theorem 1.9).

Remark 6.2. In the case $\alpha = 1/2$, one can consider that all the terms involving K are multiplied by $\sqrt{\varepsilon}$. As a first consequence, it is enough to work in Σ^2 to prove that the term involving $\tilde{W}_j^\varepsilon$ is negligible. By working in Σ^2, we only need to differentiate V_j^ε and K_j^ε twice, hence the regularity assumption in Theorem 1.5. Finally, since the phase shift relating $\tilde{u}_j^\varepsilon$ and u_j^ε is multiplied by $\sqrt{\varepsilon}$, it is $\mathcal{O}(\sqrt{\varepsilon})$, as opposed to $\mathcal{O}(1)$ in the case $\alpha = 0$.

7. The bootstrap argument

In this section, we prove Theorem 6.1. More precisely, we focus on (6.8), in view of the discussion at the end of Section 6.

In Section 6, we have essentially resumed the computations of Section 2, up to two aspects:

- We have not used Taylor's formula for V and K.
- The terms θ_j^ε do not appear in the case of the u_j's (replacing u_j^ε with u_j in the expression of θ_j^ε yields $\theta_j^\varepsilon = 0$).

In Section 3, we have seen that the analogue of the term W_j^ε (or, equivalently, $\tilde{W}_j^\varepsilon$) is negligible in the limit $\varepsilon \to 0$. These properties can be summarized as follows: the functions u_1 and u_2 solve

$$i\partial_t u_j + \frac{1}{2}\Delta u_j = V_j^\varepsilon u_j + \left(K_{j,\mathrm{diag}}^\varepsilon * |u_j|^2\right) u_j + \left(K_{j,\mathrm{off}}^\varepsilon * |u_{j+1}|^2\right) u_j + \rho_j^\varepsilon, \tag{7.1}$$

where ρ_j^ε is given by the formula:

$$\rho_j^\varepsilon = \left(V_j^0 - V_j^\varepsilon\right) u_j + \left(\left(K^\varepsilon_{j,\rm diag} - K^0_{j,\rm diag}\right) * |u_j|^2\right) u_j \\ + \left(\left(K^\varepsilon_{j,\rm off} - K^0_{j,\rm off}\right) * |u_{j+1}|^2\right) u_j,$$

where V_j^0, K_j^0 are given by (6.3)–(6.5) with $\varepsilon = 0$. We infer from (6.3)–(6.5) and Proposition 1.8 that for all $T > 0$, there exists $C > 0$ independent of $\varepsilon \in (0, 1]$ such that

$$\sup_{t\in[0,T]} \|\rho_j^\varepsilon(t)\|_{\Sigma^3} \leqslant C\sqrt{\varepsilon}.$$

Since the bootstrap argument runs in Σ^3, it is natural to work with such an estimate for the source term. This in turn imposes to work with $a_j \in \Sigma^6$, as well as V and K as in Theorem 6.1.

Set $w_j^\varepsilon = \tilde u_j^\varepsilon - u_j$: subtracting (7.1) from (6.7), we see that the error satisfies the coupled system, for $j = 1, 2$,

$$\begin{cases} i\partial_t w_j^\varepsilon + \dfrac{1}{2}\Delta w_j^\varepsilon = V_j^\varepsilon w_j^\varepsilon + \left(K^\varepsilon_{j,\rm diag} * |\tilde u_j^\varepsilon|^2\right)\tilde u_j^\varepsilon - \left(K^\varepsilon_{j,\rm diag} * |u_j|^2\right) u_j \\ \qquad\qquad + \left(K^\varepsilon_{j,\rm off} * |\tilde u_{j+1}^\varepsilon|^2\right)\tilde u_j^\varepsilon - \left(K^\varepsilon_{j,\rm off} * |u_{j+1}|^2\right) u_j \\ \qquad\qquad + \dfrac{1}{\varepsilon}\left(2\,\mathrm{Re}\,\tilde W_j^\varepsilon\right)\tilde u_j^\varepsilon - \rho_j^\varepsilon, \end{cases} \tag{7.2}$$

with initial data $w^\varepsilon_{j|t=0} = 0$. Fix $T > 0$ once and for all in the course of the proof. By Proposition 1.8, there exists $C_0 > 0$ such that

$$\sup_{t\in[0,T]} \|u_1(t)\|_{\Sigma^3} + \sup_{t\in[0,T]} \|u_2(t)\|_{\Sigma^3} \leqslant C_0.$$

Since $w^\varepsilon_{j|t=0} = 0$ and $\tilde u_j^\varepsilon \in C([0,\tau^\varepsilon];\Sigma^3)$ for some τ^ε, we can find $t^\varepsilon > 0$ such that

$$\|w_1^\varepsilon(t)\|_{\Sigma^3} + \|w_2^\varepsilon(t)\|_{\Sigma^3} \leqslant C_0 \tag{7.3}$$

for $0 \leqslant t \leqslant t^\varepsilon$. So long as (7.3) holds, we perform energy estimates, to show that (6.8) is true, with a constant C independent of ε. It will follow that up to choosing $\varepsilon \in (0, \varepsilon_0]$ with $\varepsilon_0 > 0$ sufficiently small, (7.3) holds for $t \in [0, T]$, which yields Theorem 6.1.

Notation. For two positive numbers a^ε and b^ε, the notation $a^\varepsilon \lesssim b^\varepsilon$ means that there exists $C > 0$ *independent of* ε such that for all $\varepsilon \in (0, 1]$, $a^\varepsilon \leqslant C b^\varepsilon$.

Note that so long as (7.3) holds, similarly to the case of I_j^ε, Proposition 3.1 implies

$$\left\|\tilde W_j^\varepsilon(t)\right\|_{W^{3,\infty}} \lesssim \varepsilon^{3/2},$$

hence

$$\left\|\frac{1}{\varepsilon}\left(2\,\mathrm{Re}\,\tilde W_j^\varepsilon\right)\tilde u_j^\varepsilon\right\|_{\Sigma^3} \lesssim \sqrt{\varepsilon}.$$

Therefore, the last line in (7.2), viewed as a source term, is $\mathcal{O}(\sqrt{\varepsilon})$ in Σ^3, so long as (7.3) holds. The other terms in (7.2) can then be considered as linear terms, in view of the application of Gronwall's Lemma.

We write

$$\begin{aligned}\left(K^\varepsilon_{j,\rm diag} * |\tilde u^\varepsilon_j|^2\right)\tilde u^\varepsilon_j - \left(K^\varepsilon_{j,\rm diag} * |u_j|^2\right)u_j &= \left(K^\varepsilon_{j,\rm diag} * |\tilde u^\varepsilon_j|^2\right)w^\varepsilon_j \\ &\quad + \left(K^\varepsilon_{j,\rm diag} * \left(|\tilde u^\varepsilon_j|^2 - |u_j|^2\right)\right)u_j \\ &= \left(K^\varepsilon_{j,\rm diag} * |\tilde u^\varepsilon_j|^2\right)w^\varepsilon_j \\ &\quad + \left(K^\varepsilon_{j,\rm diag} * \left(|w^\varepsilon_j|^2 + 2\,\mathrm{Re}\,\bar u_j w^\varepsilon_j\right)\right)u_j,\end{aligned}$$

and a similar relation for the off-diagonal kernel. We develop the general convolution, where K^ε is of the form (6.4):

$$\begin{aligned}(K^\varepsilon * f)\,g &= \left(\iint_0^1 \left\langle y-z, \nabla^2 K\left(\theta(y-z)\sqrt{\varepsilon}\right)(y-z)\right\rangle (1-\theta)d\theta f(z)dz\right) g \\ &= \left\langle y, \left(\iint_0^1 (1-\theta)\nabla^2 K\left(\theta(y-z)\sqrt{\varepsilon}\right)d\theta f(z)dz\right) y\right\rangle g \\ &\quad + \left(\iint_0^1 \left\langle z, \nabla^2 K\left(\theta(y-z)\sqrt{\varepsilon}\right) z\right\rangle (1-\theta)d\theta f(z)dz\right) g \\ &\quad - 2\left\langle y, \iint_0^1 (1-\theta)\nabla^2 K\left(\theta(y-z)\sqrt{\varepsilon}\right) z d\theta f(z)dz\right\rangle g.\end{aligned}$$

The same computation is available for (6.5), with heavier notations, so we leave it out. From this we readily infer

$$\left\|\left(K^\varepsilon_{j,\rm diag} * \left(|w^\varepsilon_j|^2 + 2\,\mathrm{Re}\,\bar u_j w^\varepsilon_j\right)\right)u_j\right\|_{\Sigma^3} \lesssim \|w^\varepsilon_j\|^2_{\Sigma^3} + \|w^\varepsilon_j\|_{\Sigma^3} \lesssim \|w^\varepsilon_j\|_{\Sigma^3}$$

where we have used Proposition 1.8, Cauchy–Schwarz inequality, and (7.3) for the last estimate. We can infer an L^2 estimate for w^ε_j: since all the terms of the form $K^\varepsilon_j * |\tilde u^\varepsilon|^2$ are real valued, the standard energy estimate yields

$$\begin{aligned}\|w^\varepsilon_j(t)\|_{L^2} &\leqslant \int_0^t \left\|\left(K^\varepsilon_{j,\rm diag} * \left(|w^\varepsilon_j|^2 + 2\,\mathrm{Re}\,\bar u_j w^\varepsilon_j\right)\right)u_j\right\|_{L^2} ds \\ &\quad + \int_0^t \left\|\left(K^\varepsilon_{j,\rm off} * \left(|w^\varepsilon_{j+1}|^2 + 2\,\mathrm{Re}\,\bar u_{j+1} w^\varepsilon_{j+1}\right)\right)u_j\right\|_{L^2} ds \\ &\quad + \int_0^t \left\|\frac{1}{\varepsilon}\left(2\,\mathrm{Re}\,\tilde W^\varepsilon_j\right)\tilde u^\varepsilon_j\right\|_{L^2} ds + \int_0^t \|\rho^\varepsilon_j(s)\|_{L^2} ds \\ &\lesssim \int_0^t \left(\|w^\varepsilon_j(s)\|_{\Sigma^3} + \|w^\varepsilon_{j+1}(s)\|_{\Sigma^3}\right) ds + \int_0^t \sqrt{\varepsilon} ds.\end{aligned}$$

To pass from this L^2 estimate to a Σ^3 estimate, we have to assess the action of the operators of multiplication by y_j and ∇_{y_j} on (7.2). First, ∇_{y_j} commutes with the left hand side of (7.2), but not with the right hand side. We write

$$\partial^3_{k\ell m}\left(V^\varepsilon_j w^\varepsilon_j\right) = V^\varepsilon_j \partial^3_{k\ell m} w^\varepsilon_j + \sum_{\substack{0\leqslant|\alpha|\leqslant 2\\ |\beta| = 3-|\alpha|}} c(\alpha,k,\ell,m)\partial^\beta V^\varepsilon_j \partial^\alpha w^\varepsilon_j.$$

The first term vanishes in an L^2 estimate of $\partial^3_{k\ell m} w^\varepsilon_j$, and in view of (6.2), for all multi-indices α,β with $0\leqslant|\alpha|\leqslant 2$ and $|\beta| = 3-|\alpha|$,

$$\left\|\partial^\beta V^\varepsilon_j \partial^\alpha w^\varepsilon_j\right\|_{L^2} \lesssim \|w^\varepsilon_j\|_{\Sigma^3}.$$

Remark 7.1. The presence of the potential V^ε_j, which is morally a time dependent harmonic potential, forces us to work in Σ^3, and not simply in $H^3(\mathbf{R}^d)$: this is a standard feature

of such potentials, whose associated dynamics consists of rotations in phase space, so the regularity/decay of the functions must be the same in space and in frequency.

The terms $\left(K^\varepsilon_{j,\rm diag} * |\tilde u^\varepsilon_j|^2\right) w^\varepsilon_j$ and $\left(K^\varepsilon_{j,\rm off} * |\tilde u^\varepsilon_{j+1}|^2\right) w^\varepsilon_j$ are treated similarly, and produce a term of the form real$\times\partial^3_{k\ell m} w^\varepsilon_j$, plus a term controlled in L^2 by $\|w^\varepsilon_j\|_{\Sigma^3}$, so long as (7.3) holds.

On the other hand, the multiplication by y_j commutes with the right hand side of (7.2), but not with the left hand side:

$$\left[i\partial_t + \frac{1}{2}\Delta, y\right] = \nabla,$$

so the commutation errors for the equation satisfied by $|y_j|^3 w^\varepsilon_j$ consists of a linear combination, with constant coefficients, of terms of the form $y_j^\alpha \partial^\beta w^\varepsilon_j$, with $|\alpha|+|\beta|=3$. We end up with, so long as (7.3) holds:

$$\|w^\varepsilon_j(t)\|_{\Sigma^3} \lesssim \int_0^t \left(\|w^\varepsilon_j(s)\|_{\Sigma^3} + \|w^\varepsilon_{j+1}(s)\|_{\Sigma^3}\right) ds + \int_0^t \sqrt{\varepsilon} ds.$$

Gronwall's Lemma yields (6.8), hence Theorem 6.1.

8. Second order expansion and limiting phase shifts

In view of Theorem 6.1, the phase shifts θ^ε_j are such that $\dot\theta^\varepsilon_j$ are bounded on $[0,T]$, uniformly in $\varepsilon \in (0,\varepsilon_0]$, since $|u^\varepsilon_j|^2 = |\tilde u^\varepsilon_j|^2 = |u_j|^2 + \mathcal{O}(\sqrt{\varepsilon})$. To study the limit of θ^ε_j as $\varepsilon\to 0$, we need to perform a second order expansion of $(\tilde u^\varepsilon_1, \tilde u^\varepsilon_2)$ as $\varepsilon \to 0$, to understand the contribution of order $\sqrt{\varepsilon}$. Therefore, we seek

$$\tilde u^\varepsilon_j = u_j + \sqrt{\varepsilon} u_j^{(1)} + \mathcal{O}(\varepsilon). \tag{8.1}$$

Remark 8.1. An error term of order $\mathcal{O}(\varepsilon)$ is natural, since one could actually seek a more general asymptotic expansion to arbitrary order, of the form

$$\tilde u^\varepsilon_j = u_j + \sum_{\ell=1}^N \varepsilon^{\ell/2} u_j^{(\ell)} + \mathcal{O}\left(\varepsilon^{(N+1)/2}\right). \tag{8.2}$$

Resuming the arguments presented in Section 6, we see that formally, the last line in (6.6) is $\mathcal{O}(\varepsilon^\infty)$, if we work with an infinite regularity. To get a second order approximation of $\tilde u^\varepsilon_j$, we simply need to prove that this term is $\mathcal{O}(\varepsilon)$, but we can certainly not perform the study with only an $\mathcal{O}(\sqrt{\varepsilon})$ information like we did in order to establish Theorem 6.1. To compute the limit of θ^ε_j, we need to establish the asymptotic behavior of $\tilde u^\varepsilon_j$ up to $\mathcal{O}(\varepsilon)$ in Σ, and not only in L^2, so we make an extra regularity assumption. We remark that if in Theorem 6.1, we require $a_1, a_2 \in \Sigma^7$, with

$$\begin{aligned} &V \in C^7(\mathbf{R}_+\times\mathbf{R}^d;\mathbf{R}), \quad \text{and} \quad \partial^\beta_x V \in L^\infty\left(\mathbf{R}_+\times\mathbf{R}^d\right), \quad 2\leqslant|\beta|\leqslant 7,\\ &K \in W^{7,\infty}(\mathbf{R}^d;\mathbf{R}),\end{aligned}$$

then the conclusions of Theorem 6.1 can be replaced by: $(\tilde u^\varepsilon_1, \tilde u^\varepsilon_2) \in C([0,T];\Sigma^4)^2$ and

$$\sup_{t\in[0,T]} \|\tilde u^\varepsilon_1(t) - u_1(t)\|_{\Sigma^4} + \sup_{t\in[0,T]} \|\tilde u^\varepsilon_2(t) - u_2(t)\|_{\Sigma^4} \leqslant C\sqrt{\varepsilon}.$$

In particular, $(\tilde u^\varepsilon_1, \tilde u^\varepsilon_2) \in C([0,T];\Sigma^4)^2$ *uniformly* for $\varepsilon \in (0,\varepsilon_0]$. Thanks to Proposition 3.1, this enables us to claim that in (6.7),

$$\left\|\tilde W^\varepsilon_j(t)\right\|_{W^{3,\infty}} \lesssim \varepsilon^2,$$

hence

$$\left\|\frac{1}{\varepsilon}\left(2\operatorname{Re}\tilde{W}_j^\varepsilon\right)\tilde{u}_j^\varepsilon\right\|_{\Sigma^3}\lesssim \varepsilon.$$

To derive an equation for the corrector $u_j^{(1)}$, we plug (8.1) into (6.7), and discard all the terms which are, at least formally, $\mathcal{O}(\varepsilon)$, including thus the last line. The term corresponding to the power $\sqrt{\varepsilon}$ yields:

$$\begin{aligned}
i\partial_t u_j^{(1)}+\frac{1}{2}\Delta u_j^{(1)} &= V_j^0 u_j^{(1)}+\left(K^0_{j,\mathrm{diag}}*|u_j|^2\right)u_j^{(1)}+\left(K^0_{j,\mathrm{off}}*|u_{j+1}|^2\right)u_j^{(1)}\\
&\quad +2\left(K^0_{j,\mathrm{diag}}*\operatorname{Re}\left(\overline{u}_j u_j^{(1)}\right)\right)u_j+2\left(K^0_{j,\mathrm{off}}*\operatorname{Re}\left(\overline{u}_{j+1}u_{j+1}^{(1)}\right)\right)u_j\\
&\quad +\mathcal{V}_j u_j+\left(\mathcal{K}_{j,\mathrm{diag}}*|u_j|^2\right)u_j+\left(\mathcal{K}_{j,\mathrm{off}}*|u_{j+1}|^2\right)u_j,
\end{aligned}\tag{8.3}$$

with Cauchy data $u^{(1)}_{j|t=0}=0$, where we have denoted the third order Taylor expansions

$$\begin{aligned}
\mathcal{V}_j(t,y)&=\frac{1}{6}\nabla^3 V\left(t,q_j(t)\right)y\cdot y\cdot y,\\
\mathcal{K}_{j,\mathrm{diag}}(y)&=\frac{1}{6}\nabla^3 K(0)y\cdot y\cdot y,\\
\mathcal{K}_{j,\mathrm{off}}(t,y)&=\frac{1}{6}\nabla^3 K\left(q_j(t)-q_{j+1}(t)\right)y\cdot y\cdot y.
\end{aligned}$$

These equations are naturally linear in the unknown $(u_1^{(1)},u_2^{(1)})$. In view of Proposition 1.8, the last line in (8.3), which corresponds to a source term, belongs to $C(\mathbf{R}_+;\Sigma^4)$. This non-trivial source term makes $u_j^{(1)}$ non-zero. Even though (8.3) is a linear system, it seems easier to prove that it has a unique solution, by proceeding in the same way as in the proof of Proposition 1.8 (see Section 5). We have:

Proposition 8.2. *Suppose that* $a_1,a_2\in\Sigma^7$, *and*

$$\begin{aligned}
&V\in C^7(\mathbf{R}_+\times\mathbf{R}^d;\mathbf{R}),\quad \textit{and}\quad \partial_x^\beta V\in L^\infty\left(\mathbf{R}_+\times\mathbf{R}^d\right),\quad 2\leqslant|\beta|\leqslant 7,\\
&K\in W^{7,\infty}(\mathbf{R}^d;\mathbf{R}).
\end{aligned}$$

Then (8.3) *has a unique solution* $\left(u_1^{(1)},u_2^{(1)}\right)\in C(\mathbf{R}_+;\Sigma^4)$.

Denote by $v_j^\varepsilon=u_j+\sqrt{\varepsilon}u_j^{(1)}$ the second order approximate solution, and by $\tilde{w}_j^\varepsilon=\tilde{u}_j^\varepsilon-v_j^\varepsilon$ the corresponding error term. It satisfies $\tilde{w}^\varepsilon_{j|t=0}=0$, and

$$\left\{\begin{aligned}
i\partial_t\tilde{w}_j^\varepsilon+\frac{1}{2}\Delta\tilde{w}_j^\varepsilon &= V_j^\varepsilon\tilde{w}_j^\varepsilon+\left(K^\varepsilon_{j,\mathrm{diag}}*|\tilde{u}_j^\varepsilon|^2\right)\tilde{u}_j^\varepsilon-\left(K^\varepsilon_{j,\mathrm{diag}}*|v_j^\varepsilon|^2\right)v_j^\varepsilon\\
&\quad+\left(K^\varepsilon_{j,\mathrm{off}}*|\tilde{u}_{j+1}^\varepsilon|^2\right)\tilde{u}_j^\varepsilon-\left(K^\varepsilon_{j,\mathrm{off}}*|v_{j+1}^\varepsilon|^2\right)v_j^\varepsilon\\
&\quad+\frac{1}{\varepsilon}\left(2\operatorname{Re}\tilde{W}_j^\varepsilon\right)\tilde{u}_j^\varepsilon-\tilde{\rho}_j^\varepsilon,
\end{aligned}\right.$$

where the new source term is such that

$$\sup_{t\in[0,T]}\|\tilde{\rho}_j^\varepsilon(t)\|_\Sigma\leqslant C\varepsilon.$$

Resuming the energy estimates used in Section 7, we infer:

Proposition 8.3. *Let $T>0$. Under the assumptions of Proposition 8.2, there exists $\varepsilon_0>0$ such that for $\varepsilon\in(0,\varepsilon_0]$,* (6.7) *has a unique solution $(\tilde u_1^\varepsilon,\tilde u_2^\varepsilon)\in C([0,T];\Sigma^4)^2$. Moreover, there exists C independent of $\varepsilon\in(0,\varepsilon_0]$ such that*

$$\sup_{t\in[0,T]}\left\|\tilde u_1^\varepsilon(t)-u_1(t)-\sqrt{\varepsilon}u_1^{(1)}(t)\right\|_\Sigma+\sup_{t\in[0,T]}\left\|\tilde u_2^\varepsilon(t)-u_2(t)-\sqrt{\varepsilon}u_2^{(1)}(t)\right\|_\Sigma\leqslant C\varepsilon.$$

Note that unlike in the proof of Theorem 6.1, no bootstrap argument is needed at this stage, since we already have uniform estimates for $\tilde u_j^\varepsilon,u_j,u_j^{(1)}$ in $C([0,T];\Sigma^4)$. We readily infer:

$$\theta_j^\varepsilon(t)=\theta_j(t)+\mathcal{O}\left(\sqrt{\varepsilon}\right)\quad\text{ in }L^\infty([0,T]),$$

where θ_j is given by

$$\begin{aligned}\theta_j(t)&=\int_0^t\nabla K(0)\cdot\left(2\operatorname{Re}\int z\overline{u}_j(s,z)u_j^{(1)}(s,z)dz\right)ds\\&\quad+\int_0^t\nabla K(q_j(s)-q_{j+1}(s))\cdot\left(2\operatorname{Re}\int z\overline{u}_{j+1}(s,z)u_{j+1}^{(1)}(s,z)dz\right)ds.\end{aligned}\tag{8.4}$$

We have obviously $\theta_j\in C^1([0,T])$, and $\theta_j(0)=\dot\theta_j(0)=0$. To see that $\theta_j\in C^2([0,T])$, in view of the Cauchy–Schwarz inequality, and since $u_j,u_j^{(1)}\in C([0,T];\Sigma)$, it suffices that verify that $u_j,u_j^{(1)}\in C^1([0,T];L^2)$. This property is a straightforward consequence of Equations (1.13) and (8.3), in view of the regularity of u_j and $u_j^{(1)}$. This completes the proof of Theorem 1.9.

To conclude, we check that the phase shifts θ_j are non-trivial in general, by computing their initial second order derivatives: since $u^{(1)}_{j|t=0}=0$,

$$\begin{aligned}\ddot\theta_j(0)&=\nabla K(0)\cdot\left(2\operatorname{Re}\int z\overline{a}_j(z)\partial_t u_j^{(1)}(0,z)dz\right)\\&\quad+\nabla K(q_j(0)-q_{j+1}(0))\cdot\left(2\operatorname{Re}\int z\overline{a}_{j+1}(z)\partial_t u_{j+1}^{(1)}(0,z)dz\right).\end{aligned}$$

From (8.3), we have

$$i\partial_t u_j^{(1)}(0,y)=\left(\mathcal{V}_j(0,y)+\mathcal{K}_{j,\mathrm{diag}}*|a_j|^2+\mathcal{K}_{j,\mathrm{off}}*|a_{j+1}|^2\right)a_j(y),$$

so the first line in the expression for $\ddot\theta_j(0)$ is zero, and

$$\begin{aligned}\ddot\theta_j(0)&=\nabla K(q_j(0)-q_{j+1}(0))\cdot\left(\int z\mathcal{V}_j(0,z)2\operatorname{Im}\left(\overline{a}_{j+1}a_j\right)(z)dz\right)\\&\quad+\nabla K(q_j(0)-q_{j+1}(0))\cdot\left(\int\left(\mathcal{K}_{j,\mathrm{diag}}*|a_j|^2\right)2\operatorname{Im}\left(\overline{a}_{j+1}a_j\right)(z)dz\right)\\&\quad+\nabla K(q_j(0)-q_{j+1}(0))\cdot\left(\int\left(\mathcal{K}_{j,\mathrm{off}}*|a_{j+1}|^2\right)2\operatorname{Im}\left(\overline{a}_{j+1}a_j\right)(z)dz\right).\end{aligned}$$

Therefore in general $\theta_j\not\equiv 0$.

Remark 8.4 (Instability). The fact that it is necessary to analyze an $\mathcal{O}(\sqrt{\varepsilon})$ correction to (u_1,u_2) to compute (θ_1,θ_2) implies the existence of instabilities at the semi-classical level. Typically, a perturbation of the initial data at order ε^γ with $0<\gamma<1/2$ will affect the leading order behavior of u^ε in L^2 (for the strong topology) for some time $0<t^\varepsilon\to 0$. On the other hand, since the θ_j's are purely time dependent, the Wigner measure are not

affected by this phenomenon. Since the approach to describe this instability is the same as in [10], we simply refer to that paper for more details.

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